Understanding the invisible through numerical simulation of wave propagation

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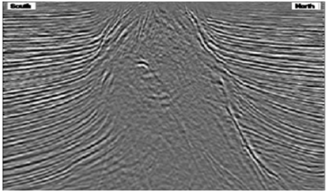
1 Introduction

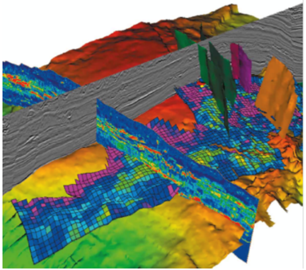
Broad scientific context

Describe a place with exactness from more or less numerous and precise memories, or guessing the content and internal structures of an object after having observed it only partially, without ever touching it because it is inaccessible or very fragile?

1. **Wave propagation is helping**
2. **Waves are very sensitive to any change in the propagation medium.**



(a) Seismogram.



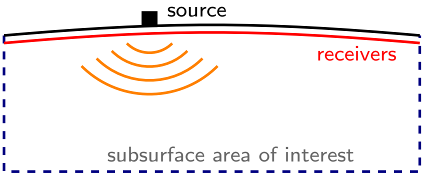
(b) Reservoir model.

Inverse problems

Basically, inverse wave problems are composed of:

1. Emitting sources that will propagate through the medium and recording the reflected waves on a set of receivers; acquisition/ forward problem
2. From the acquisitions, find the propagation medium; inverse problem/backward problem

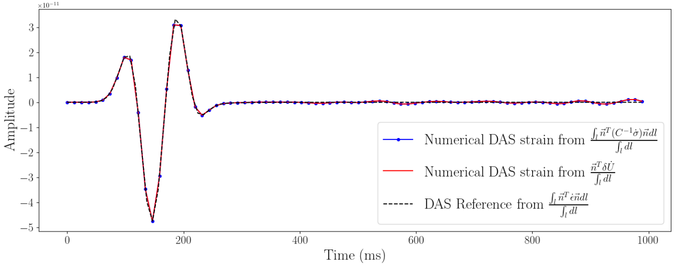
Example: Seismic imaging for the **Reconstruction/Monitoring** of subsurface Earth properties



1. **Accurate simulation of wave propagation in large-scale complex media,**
2. **Efficient procedure for nonlinear reconstruction of properties.**

Numerical data match real data

Compare data with simulations: computationally and possibly timely expensive



Comparison of observation and numerical result

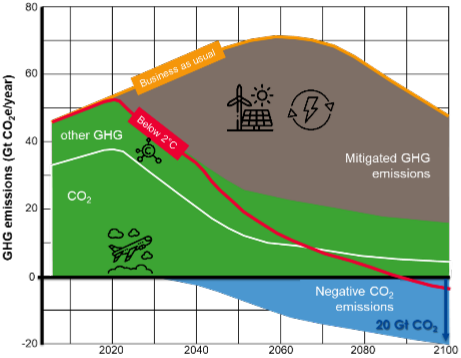
..

Plan

2 Energy Geophysics

Access to energy resources

- Hydrocarbons
- Geothermal
- Hydrogen



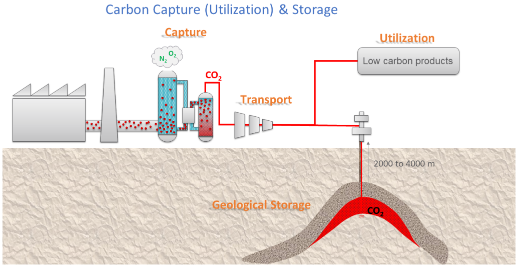
Source: The Emissions Gap Report 2017. United Nations Environment Programme (UNEP)

Facilitate safe carbon capture, utilization and storage - CCUS

- CO_2 emissions: leading cause of climate change;
- Geological storage of CO_2: important tool for the stabilization of atmospheric greenhouse gas concentrations;
- CO_2 is injected into underground geological formations; Safe, permanent, and effective.

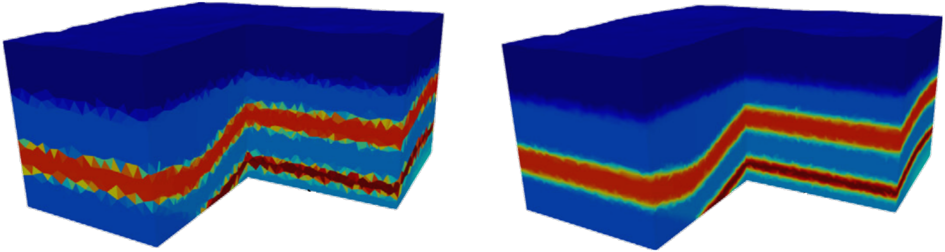
How do we ensure the safety and sustainability of storage?

That's where seismic monitoring comes into play.



Research routine: propagation domains

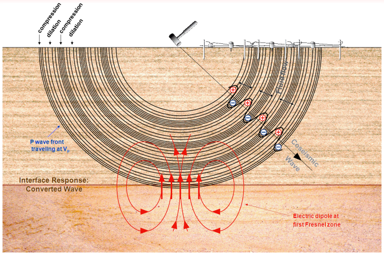
- 3D large domains
- topography, heterogeneity
- a network of sources whose number is of the order of several thousands

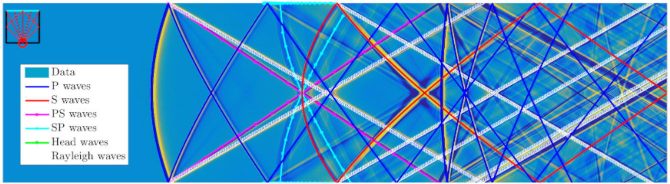


Parameterization matters

Research routine: wave equations

- Acoustic wave equation,
- Elastic wave equation,
- Electromagnetic wave equation,
- Couplings





Waves in solid media

Equations 2/2

Acoustic wave equation, time and frequency domains:

$$\begin{cases} \rho \partial_t \mathbf{v}(\mathbf{x}, t) = -\nabla p(\mathbf{x}, t), \\ \\ \dfrac{1}{c^2 \rho} \partial_t p(\mathbf{x}, t) + \boldsymbol{\nabla} \cdot \mathbf{v}(\mathbf{x}, t) = 0. \end{cases}$$

$$\begin{cases} -\mathrm{i}\,\omega \rho \mathbf{v}(\mathbf{x}, \omega) = -\nabla p(\mathbf{x}, \omega), \\ \\ -\dfrac{1}{c^2 \rho} \mathrm{i}\omega p(\mathbf{x}, \omega) + \boldsymbol{\nabla} \cdot \mathbf{v}(\mathbf{x}, \omega) = 0. \end{cases}$$

Elasto-dynamic equations, time and frequency domains:

$$\begin{cases} \rho \partial_t \mathbf{v}(\boldsymbol{x}, t) = \boldsymbol{\nabla} \cdot \underline{\underline{\sigma}}(\boldsymbol{x}, t), \\ \\ \partial_t \underline{\underline{\sigma}}(\boldsymbol{x}, t) = \underline{\underline{C}}(\boldsymbol{x})(\underline{\epsilon}(\mathbf{v})). \end{cases}$$

$$\begin{cases} -\mathrm{i}\omega \rho \mathbf{v}(\boldsymbol{x}, \omega) = \boldsymbol{\nabla} \cdot \underline{\underline{\sigma}}(\boldsymbol{x}, \omega), \\ \\ -\mathrm{i}\omega \underline{\underline{\sigma}}(\boldsymbol{x}, \omega) = \underline{\underline{C}}(\boldsymbol{x})(\underline{\epsilon}(\mathbf{v})). \end{cases}$$

Equations 2/2

Each approach has pros and cons

Time-domain formulation

- Using data is straightforward
- Matrix-free implementation relieves memory,
- frequency-dependent parameters,
- adjoint of the discrete problem can differ from discrete adjoint, additional developments are required,
- multi-sources

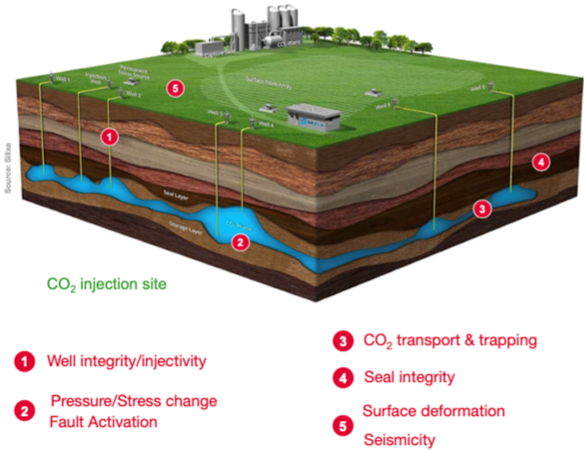
Time-harmonic formulation

- Easily handle attenuation,
- multi-sources with direct solver,
- reuse matrix factorization for adjoint-problem in inversion,
- memory cost for matrix factorization with direct solver,

Modelling and simulation challenges 1/2

A multi-physics problem and...

- ✓ CO2 sequestration and monitoring are more and more recognized as a key element in the path towards energy decarbonization
- ✓ CO2 sequestration and monitoring is an excellent example gathering the leading-edge technology of many different domain to help in the prediction of the plume evolution:
  - ✓ Flow and geo-mechanical simulation,
  - ✓ Gravimetry,
  - ✓ Seismic modelling and inverse problem, monitoring acquisition technology,
  - ✓ In situ data visualization and analysis,
  - ✓ Machine learning
  - ✓ ...

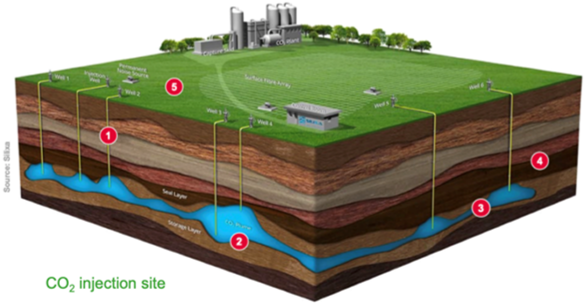


Modelling and simulation challenges 2/2

HPC Issue

- ✓ **Limitations:**
  - ✓ **Multiphysics: geomechanic+Flow+Seismic**
  - ✓ **Large Scale: 98% storage in Aquifer**
  - ✓ **Long Term Simulation: post injection matters**
- ✓ **Solutions:**
  - ✓ **Fast and scalable algorithms**
  - ✓ **Perennial solutions: portability**

Target: Exascale Computers

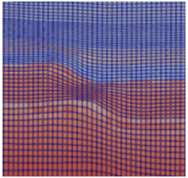


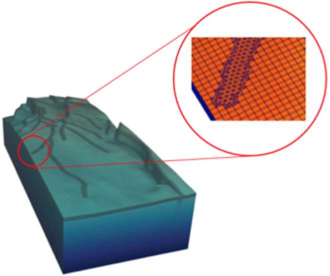
CO_2 injection site

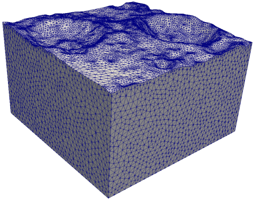
1. Well integrity/injectivity
2. Pressure/Stress change
   Fault Activation
3. CO_2 transport & trapping
4. Seal integrity
5. Surface deformation
   Seismicity

Numerical methods 1/2

- Finite Differences: implementation easy, low cost, inaccuracy for the topography
- Finite Elements: implementation possibly tricky, expensive, accurate for the topography
- Boundary integral equations: not efficient in highly heterogeneous media
- Semi-Analytical: lack of flexibility, geometrical effects, anisotropy neglected,







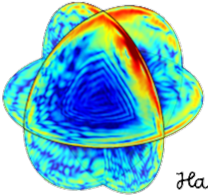
In Makutu team 2/2

- Spectral element methods (SEM)
- Discontinuous Galerkin methods (DG)
- Non polynomial basis functions in Trefftz framework

- Explicit schemes in time
- High-order
- hp-adaptivity with DG

GEOSX

Multiphysics
Simulator on HPC



Hawen

https://ffaucher.gitlab.io/hawen-website/

Plan

3. Illustration: Elastic wave propagation with HDG
   - Mathematical formulation and HDG algorithm
   - Illustration of gains

Elastic wave propagation with HDG

In collaboration with Florian Faucher and Ha Pham

Plan

3. Illustration: Elastic wave propagation with HDG
   - Mathematical formulation and HDG algorithm
   - Illustration of gains

Elastic wave problem

New sensing devices such as fiber optic measure strain (ϵ). Therefore, we want to solve for ($\boldsymbol{u}$, $\boldsymbol{\sigma}$) to have maximum accuracy rather than replacing in terms of $\boldsymbol{u}$ only.

$$\begin{cases} -\omega^2 \boldsymbol{u} - \nabla \cdot \boldsymbol{\sigma} = \boldsymbol{f}, \\ \boldsymbol{\sigma} = \frac{1}{2} \boldsymbol{C} : \epsilon, \qquad \epsilon = (\nabla \boldsymbol{u} + \nabla^T \boldsymbol{u}), \end{cases} \tag{1}$$

The physical properties describing the medium are contained in the stiffness tensor $\boldsymbol{C}$.

Time-harmonic wave problems:

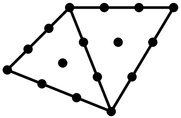
+ Easily encode the attenuation with complex-valued parameters,
+ Direct solvers allow for multiple right-hand sides once the factorization is obtained,
– Memory cost of the matrix factorization.

HDG discretization

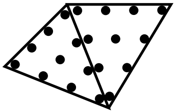
$$\begin{cases} -\omega^2 \boldsymbol{u} - \nabla \cdot \boldsymbol{\sigma} = \boldsymbol{f}\,, \\ \boldsymbol{\sigma} = \frac{1}{2}\boldsymbol{C} : \left(\nabla \boldsymbol{u} + \nabla^T \boldsymbol{u}\right)\,, \end{cases}$$

Hybridizable Discontinuous Galerkin method

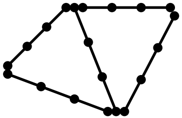
- **Static condensation** on first-order DG Formulations **without** increasing the number of unknown: The unknown of the global matrix is **only** the numerical trace $\widehat{\boldsymbol{u}}$.
- Handle **complex geometry** (topography) with *p*-adaptivity,
- Reduces the computational cost by removing inner dofs.



Finite Element



Discontinuous Galerkin



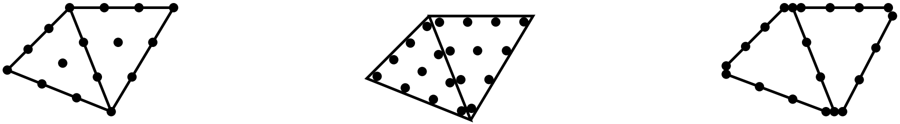
HDG

B. Cockburn J. Gopalakrishnan and R. Lazarov
Unified hybridization of discontinuous Galerkin, mixed, and continuous Galerkin methods for second order elliptic problems
SIAM Journal on Numerical Analysis (47), 2009.

HDG discretization

Hybridizable Discontinuous Galerkin method for the discretization

- Static condensation for first-order problems **without** increasing the number of unknown: The unknown of the global matrix is **only** the numerical trace $\widehat{\boldsymbol{u}}$.
- Handle **complex geometry** (topography) with p-adaptivity,
- Reduces the computational cost by removing inner dofs.



Finite Element Discontinuous Galerkin HDG

> HDG is more efficient with high-order polynomial (order > 4).
> High-order $\Rightarrow$ Large cell $\Rightarrow$ variable $\boldsymbol{C}$ within cells for resolution.

S.Du and F.J. Sayas
An Invitation to the Theory of the Hybridizable Discontinuous Galerkin Method: Projections, Estimates, Tools
Springer Nature, 2019

HDG Variational formulation (1/2): stiffness tensor version

The local problem is written on each cell K_e of the mesh, and the HDG problem is written in terms of $(\boldsymbol{u}, \boldsymbol{\sigma}, \widehat{u})$. Using test-functions (ψ, ϕ),

$$\begin{cases} \displaystyle\int_{K_e} -\omega^2 \boldsymbol{u}\,\overline{\psi} - \int_{K_e} \nabla\cdot\boldsymbol{\sigma}\,\overline{\psi} = \int_{K_e} \boldsymbol{f}\,\overline{\psi}, & \text{(2a)} \\ \displaystyle\int_{K_e} \frac{1}{2}\boldsymbol{C} : \nabla\boldsymbol{u}\overline{\phi} + \int_{K_e} \frac{1}{2}\boldsymbol{C} : \nabla^T\boldsymbol{u}\overline{\phi} - \int_{K_e} \boldsymbol{\sigma}\overline{\phi} = 0\,. & \text{(2b)} \end{cases}$$

To make appear the numerical trace $\widehat{u}$, we need to integrate by parts leading to derivative of $\boldsymbol{C}$.
$\Rightarrow$ **when $\boldsymbol{C}$ is not constant per cell, one would need to provide its derivative. . .**

Variational formulation (2/2): compliance tensor version

Using $\boldsymbol{S} = \boldsymbol{C}^{-1}$, $\begin{cases} -\omega^2 \boldsymbol{u} - \nabla \cdot \boldsymbol{\sigma} = \boldsymbol{f}\,, \\ \boldsymbol{S} : \boldsymbol{\sigma} = \frac{1}{2}(\nabla \boldsymbol{u} + \nabla^T \boldsymbol{u})\,, \end{cases}$

On each cell K_e of the mesh,

$$\begin{cases} \displaystyle\int_{K_e} -\omega^2 \boldsymbol{u}\,\overline{\psi} - \int_{K_e} \nabla \cdot \boldsymbol{\sigma}\,\overline{\psi} = \int_{K_e} \boldsymbol{f}\,\overline{\psi}, & \text{(3a)} \\ \displaystyle\int_{K_e} \frac{1}{2} \nabla \boldsymbol{u} \overline{\phi} + \int_{K_e} \frac{1}{2} \nabla^T \boldsymbol{u} \overline{\phi} - \int_{K_e} \boldsymbol{S} : \boldsymbol{\sigma} \overline{\phi} = 0\,. & \text{(3b)} \end{cases}$$

⇒ using quadrature formula, $\boldsymbol{S}$ can easily vary within cell.

Note that under isotropy, we have an explicit formulation of $\boldsymbol{S}$ from Lamé parameters.

HDG workflow in a nutshell

Unknowns are the discretized variables: $X^h = (\boldsymbol{u}^h, \boldsymbol{\sigma}^h)$ and numerical trace $\widehat{\boldsymbol{u}}^h$.

$$\begin{cases} \text{local problem on each cell } K_e : & \mathbb{A}_e X_e^h + \mathbb{C}_e \mathcal{R}_e \widehat{\boldsymbol{u}}^h = \mathbb{F}\,, \\ \text{relation for numerical trace :} & \displaystyle\sum_e \mathcal{R}_e^T \left(\mathbb{B}_e X_e^h + \mathbb{L}_e \mathcal{R}_e \widehat{\boldsymbol{u}}^h \right) = 0\,. \end{cases}$$

Reorder to write **global problem** in terms of numerical trace only

$$\sum_e \mathcal{R}_e^T \left(\mathbb{L}_e - \mathbb{B}_e \mathbb{A}_e^{-1} \mathbb{C}_e \right) \mathcal{R}_e \widehat{u}_h = -\sum_e \mathcal{R}_e^T \mathbb{B}_e \mathbb{A}_e^{-1} \mathbb{F}_e \qquad \Leftrightarrow \qquad \mathcal{A}\, \widehat{\boldsymbol{u}}_h = \mathcal{B}.$$

1. Create local matrices on each cell (embarrassingly parallel) with p-adaptivity.
2. Assemble global matrix $\mathcal{A}$.
3. Solve the large linear system $\mathcal{A}\widehat{\boldsymbol{u}}^h = \mathcal{B}$ with MUMPS (solve multiple rhs at limited cost).
4. Solve the local linear systems to obtain the volume solution $(\boldsymbol{u}^h, \boldsymbol{\sigma}^h)$: (small matrices, embarrassingly parallel, $< 2\%$ of run time).

Plan

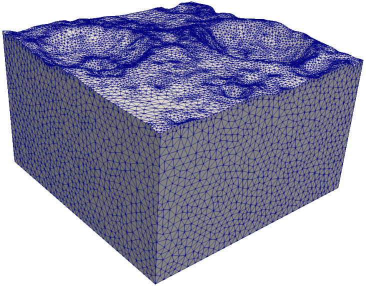
3. Illustration: Elastic wave propagation with HDG
   - Mathematical formulation and HDG algorithm
   - Illustration of gains

Elastic-wave propagation with HDG

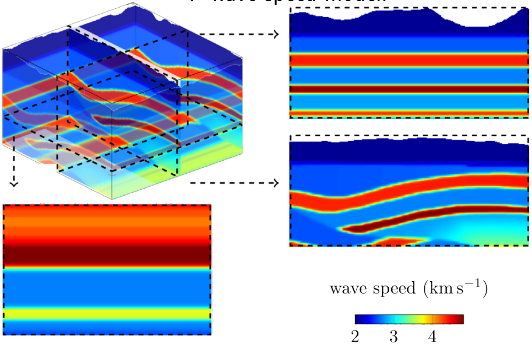
3D Model with topography, size $20\times20\times10$ km^3 with topography.

- Small cells required to accurately describe the topography, *p*-adaptivity
- Large cells elsewhere to benefit from HDG,
- models properties vary within the cell, here we use Lagrange basis per cell.

mesh



P-wave speed model.



Elastic-wave propagation with HDG

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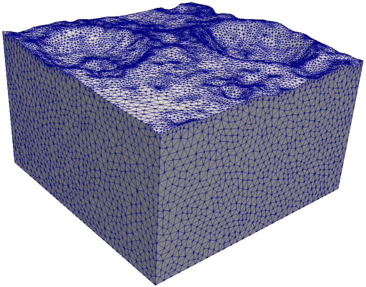
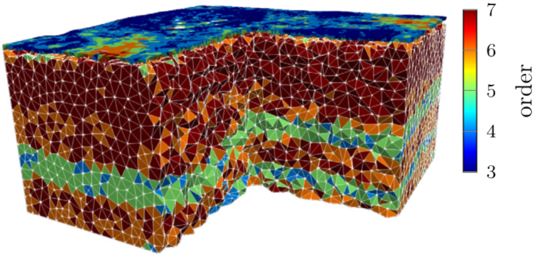


polynomial orders.



Elastic-wave propagation with HDG

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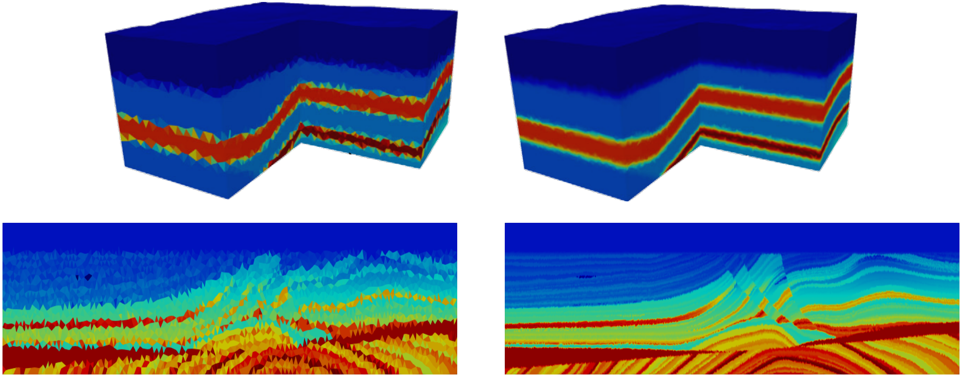
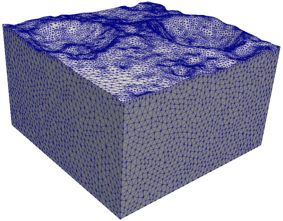


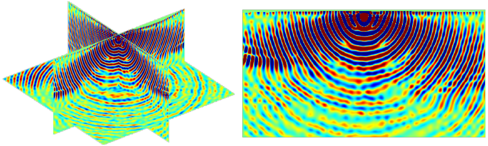
Matrix size reduction with HDG+MUMPS

3D elastic wave propagation, size 20×20×10 km^3 with topography.

Mesh using 120 000 cells

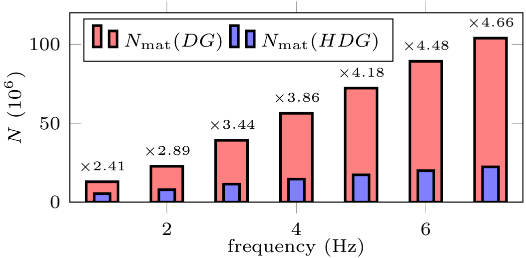


Polynomial order between 2 and 10



displacement field u_z at 4 Hz

Global matrix size with frequency



elastic simulation 7 Hz with 1600 cores **HDG+MUMPS**:

- **matrix size** $N = 22.3 \times 10^6$,
- **analysis time** 2 min 30 sec,
- **factorization time** 34 min,
- **factorization memory** 3589 GiB,
- **solve time (19 rhs)** 1 min 40 s.

Plan

4 Inverse problem

- Iterative minimization algorithm
- Numerical experiment

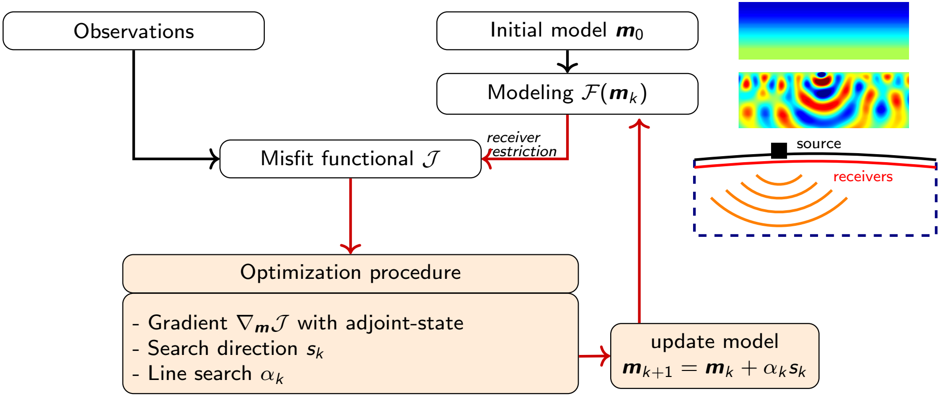
Plan

4. Inverse problem
   - Iterative minimization algorithm
   - Numerical experiment

Quantitative reconstruction algorithm: FWI

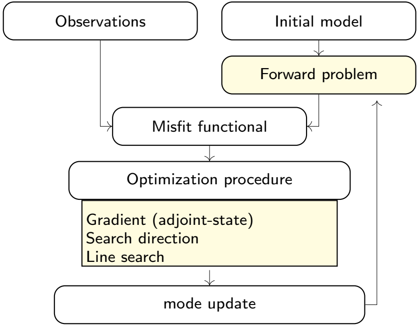
Quantitative reconstruction of properties $\boldsymbol{m} = (\lambda, \mu, \rho)$ solving iterative minimization problem.

$$\min_{\boldsymbol{m}} \mathcal{J}(\boldsymbol{m}) \quad \text{with} \quad \mathcal{J}(\boldsymbol{m}) = \mathrm{dist}\big(\mathcal{F}(\boldsymbol{m}), \boldsymbol{d}\big), \quad \mathcal{F}\text{: simulations}, \quad \boldsymbol{d}\text{: observations}.$$



Quantitative reconstruction algorithm: FWI

minimize $\quad \mathcal{J}(\boldsymbol{m}) \,=\, \mathrm{dist}\big(\,\mathcal{F}(\boldsymbol{m}),\, \boldsymbol{d}\,\big)$



1. Repeated use of forward wave propagation solver,

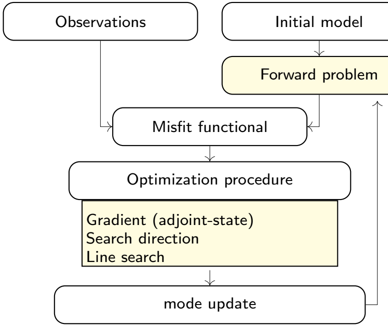
$$\begin{cases} \mathbb{A}_e X_e^h \,+\, \mathbb{C}_e \mathcal{R}_e \widehat{\boldsymbol{u}}^h \,=\, \mathbb{F}\,, & (4a) \\ \displaystyle\sum_e \mathcal{R}_e^T \Big(\mathbb{B}_e X_e^h \,+\, \mathbb{L}_e \mathcal{R}_e \widehat{\boldsymbol{u}}^h \Big) \,=\, 0\,. & (4b) \end{cases}$$

2. Adjoint-state method for gradient adapted to HDG Lagrangian written from $\mathcal{J}$ subject to (4a), (4b).

We prove that for HDG, the gradient is still computed from the the **adjoint of the direct problem**, fundamental to avoid refactorization of the global matrix.

Quantitative reconstruction algorithm: FWI

minimize $\quad \mathcal{J}(\boldsymbol{m}) = \mathrm{dist}\big(\mathcal{F}(\boldsymbol{m}), \boldsymbol{d}\big)$



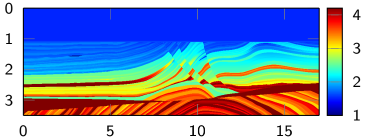
1. Repeated use of forward wave propagation solver,
2. Adjoint-state method for gradient adapted to HDG,
3. To alleviate mesh limitations, the model parameters are represented with Lagrange basis functions.
4. Inversion is carried out with respect to the weight of the Lagrange basis functions.

Plan

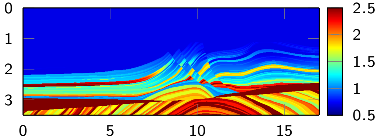
4. Inverse problem
   - Iterative minimization algorithm
   - Numerical experiment

2D experiments: Marmousi II setup

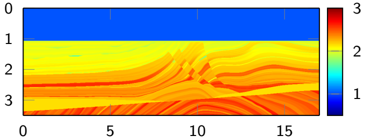
We consider the elastic isotropic Marmousi II experiment, of size 17×3.5 km^2.
Free-surface boundary condition on top and absorbing boundary conditions elsewhere.



True P-wave speed



True S-wave speed



True density

2D experiments: Marmousi II setup

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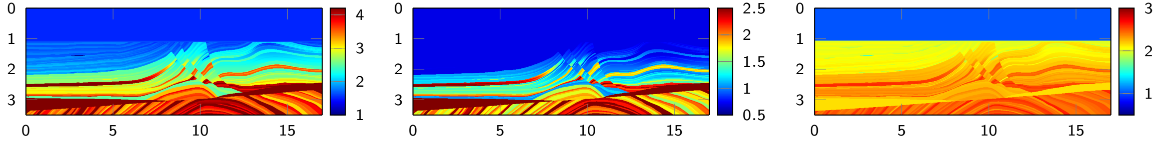
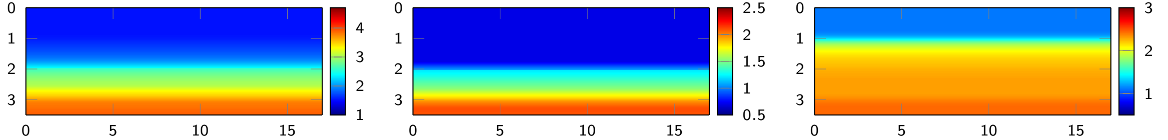


True P-wave speed True S-wave speed True density

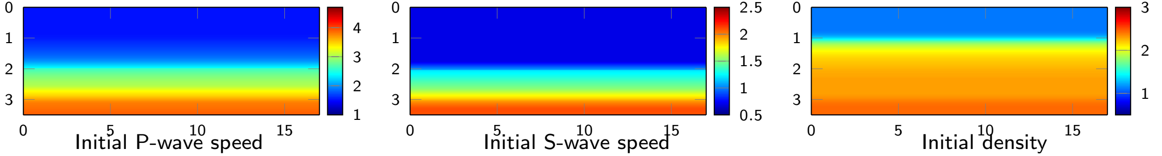
Initial models are 1D-background variation.



Initial P-wave speed Initial S-wave speed Initial density

2D experiments: Marmousi II reconstructions

- Acquisition made up of 169 sources and 849 receivers near surface.
- Reconstructions using 13 frequencies from 2 to 8 Hz, 25 iterations per frequency.
- Density is not inverted and remains in its initial value.



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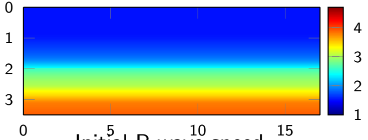
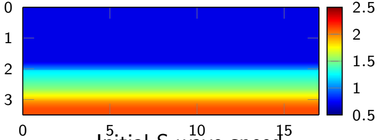
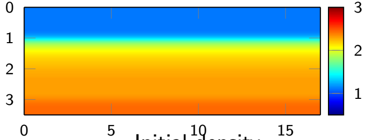


Initial P-wave speed

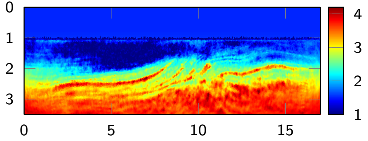


Initial S-wave speed

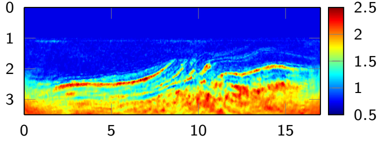


Initial density

- Reconstruction using representation in order 1 Lagrange basis per cell ($\sim 20 \times 10^3$ cells)



Reconstruction P-wave speed



Reconstruction S-wave speed

2D experiments: Marmousi II reconstructions

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- Reconstructions using 13 frequencies from 2 to 8 Hz, 25 iterations per frequency.
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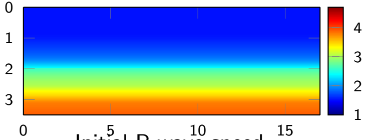
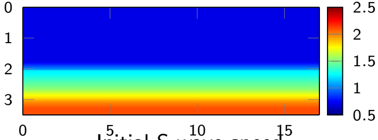
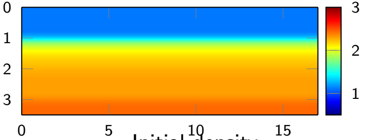


Initial P-wave speed

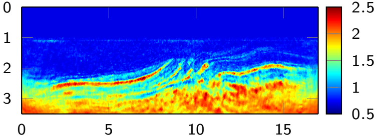


Initial S-wave speed

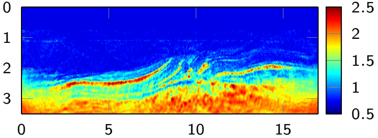


Initial density

- Computational time (18mpi $\times$ 2omp): $2{\cdot}10^4$ cells: 3h; $5{\cdot}10^4$ cells: 4h15min, i.e. **-30%**.



S-wave speed reconstruction using mesh with 20 000 cells and Lagrange basis representation,



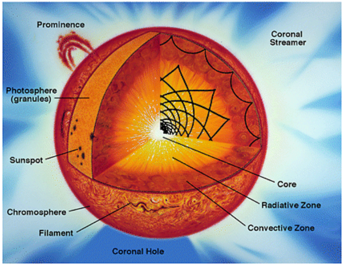
S-wave speed reconstruction using mesh with 50 000 cells piecewise-constant representation.

Plan

5 Helioseismology/asteroseismology

Helioseismic studies

- Measuring solar/star oscillations,
- Processing and averaging the observations to extract the seismic data
- Interpreting the seismic data using forward and inverse methods to estimate solar internal properties.



Solar interior

Detecting active regions on the far side of the Sun

- Of great importance for space-weather forecasts
- Large active regions that emerge on the Sun's far side will rotate into Earth's view several days later; these may trigger coronal mass ejections, which can damage satellites and spacecraft and endanger astronauts
- It is known that far-side imaging can significantly improve models of the solar wind, which plays an important role in space-weather forecasts.

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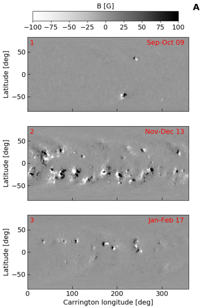

Numerical simulations of acoustic waves

Acoustic waves propagate horizontally and are trapped in the vertical direction; they connect the Sun's near and far sides. As acoustic waves travel faster in magnetized regions, they can inform us about the presence of active regions along their paths of propagation.

Two helioseismic techniques:

- Helioseismic holography: multiply the forward and backward propagated wavefields,and subtract a reference measurement for the quiet Sun.
- Time-distance helioseismology: compute the cross-covariance of the wavefield

Develop models and computational tools that are required to recover information about Sun and eventually stellar activity from observations of oscillations.

C. Lindsey and D.C. Braun, Helioseismic holography. The Astrophysical Journal, 1997

L. Gizon,H. Barucq, M. Duruflé, C.S. Hanson, M. Leguèbe, A.C. Birch, J. Chabassier, D. Fournier, T. Hohage and E. Papini, Computational helioseismology in the frequency domain: acoustic waves in axisymmetric solar models with flows. Astronomy & Astrophysics, 2017

Equations

- **Galbrun's equation** describes adiabatic wave motion subject to source F with frequency ω, on top of a time-invariant fluid background. Ignoring flows and rotation and with Cowling's approximation,

$$-\rho_0\left(\omega^2+2\,\mathrm{i}\omega\,\Gamma\right)\xi-\nabla\left[\gamma\,p_0\nabla\cdot\xi\right]+(\nabla\,p_0)(\nabla\cdot\xi)-\nabla\left(\xi\cdot\nabla\,p_0\right)+(\xi\cdot\nabla)\nabla\,p_0+\rho_0\left(\xi\cdot\nabla\right)\nabla\,\phi_0\;=\;F\,,$$

with displacement vector ξ describing the solar oscillation. The density is ρ_0, pressure p_0, adiabatic index γ, gravitational potential ϕ_0 and attenuation Γ.

H. Barucq, F. Faucher, D. Fournier, L. Gizon and H. Pham, Efficient and accurate algorithm for the full modal Green's kernel of the scalar wave equation in helioseismology. SIAM J. on Appl. Math., 2020.

H. Barucq, F. Faucher, D. Fournier, L. Gizon and H. Pham, Outgoing modal solutions for Galbrun's equation in helioseismology. J. of Differential Eq., 2021.

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  with displacement vector ξ describing the solar oscillation. The density is ρ_0, pressure p_0, adiabatic index γ, gravitational potential ϕ_0 and attenuation Γ.

- Further approximation ignoring the gravity, we obtain a **scalar-wave equation** for variable $u := \rho\, c^2\nabla\cdot\xi$ such that,

$$-\nabla\cdot\left(\frac{1}{\rho}\nabla u\right)-\frac{\omega^2+2\,i\omega\,\Gamma}{\rho\,c^2}u=f\,,\qquad \text{with sound-speed } c.$$

H. Barucq, F. Faucher, D. Fournier, L. Gizon and H. Pham, Efficient and accurate algorithm for the full modal Green's kernel of the scalar wave equation in helioseismology. SIAM J. on Appl. Math., 2020.

H. Barucq, F. Faucher, D. Fournier, L. Gizon and H. Pham, Outgoing modal solutions for Galbrun's equation in helioseismology. J. of Differential Eq., 2021.

Spherical background solar model

Model S+Atmo: exponentially decreasing density in the solar atmosphere

$$\rho(r) := \begin{cases} \rho_S(r)\,, & r \leq r_a \\ \rho_S(r_a)\; e^{-\alpha_\infty\,(r - r_a)}\,, & r > r_a \end{cases}, \qquad c(r) := \begin{cases} c_S(r), & r \leq r_a; \\ c_S(r_a), & r > r_a \end{cases}$$

with $\rho_S > \rho_0 > 0$; $c_S > c_0 > 0$, $R_\odot$ = the solar radius ($\sim 696 \times 10^3$km)

Spherical background solar model

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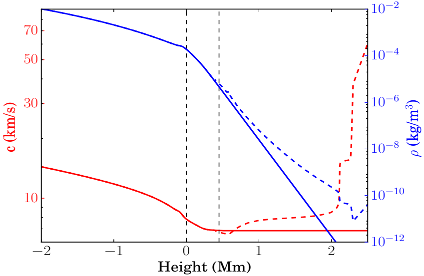
Comparison of the S+Atmo (solid) and VAL-C (dashed) atmospheric models.



Height above surface (Mm) R_h	0.5	0.556	2.543	4
scaled radius $= (R_\odot + R_h)/R_\odot$	1.0007	1.0008	1.0037	1.0058

Scalar-wave problem formulation, spherical symmetry

$$-\nabla\cdot\left(\frac{1}{\rho}\nabla u\right)-\frac{\omega^2+2\,\mathrm{i}\omega\,\Gamma}{\rho\,c^2}u=f\,.$$

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Scalar-wave problem formulation, spherical symmetry

$$-\nabla\cdot\left(\frac{1}{\rho}\nabla\mathfrak{u}\right)-\frac{\omega^2+2\,\mathrm{i}\omega\,\Gamma}{\rho\,c^2}\mathfrak{u}=\mathfrak{f}\,.$$

1. We use the Liouville transform to rewrite the problem in Schrödinger form,

With $u=\rho^{-1/2}\mathfrak{u}$ and $\alpha=-\rho'/\rho$, we obtain

$$\left(-\Delta-\frac{\omega^2+2\,\mathrm{i}\omega\,\Gamma}{c^2}+\frac{\alpha^2}{4}+\frac{\alpha'}{2}+\frac{\alpha}{r}\right)u=f\,.$$

In the atmosphere, ρ is exponentially decreasing $\Rightarrow$ α is constant.

H. Barucq, F. Faucher, D. Fournier, L. Gizon and H. Pham, Efficient and accurate algorithm for the full modal Green's kernel of the scalar wave equation in helioseismology. SIAM J. on Appl. Math., 2020.

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With $u = \rho^{-1/2}\mathfrak{u}$ and $\alpha = -\rho'/\rho$, we obtain

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In the atmosphere, ρ is exponentially decreasing $\Rightarrow$ α is constant.

2. Allows us to build the exact Dirichlet-to-Neumann map and new classes of Radiation Boundary conditions for outgoing solutions.

H. Barucq, F. Faucher, D. Fournier, L. Gizon and H. Pham, Efficient and accurate algorithm for the full modal Green's kernel of the scalar wave equation in helioseismology. SIAM J. on Appl. Math., 2020.

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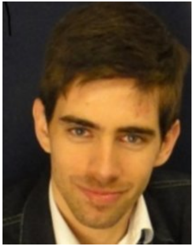
Plan

6 Illustration: Green's function computations for time-distance helioseismology

- Modal Green's kernel
- Numerical experiments
- Power spectrum, comparison with measured data
- The vector wave problem

Numerical method for computing Green's functions

In collaboration with Florian Faucher, Ha Pham, and Damien Fournier, Laurent Gizon from Max Planck Institute for Sun (MPS, Göttingen, Germany)



Cross-covariance in terms of Green's function

At frequency ω, consider the cross-covariance in Fourier space as the product of the wave field at two locations of measurement,

$$C(r_1, r_2, \omega) = \Psi^*(r_1, \omega)\Psi(r_2, \omega)$$

Here, $\Psi = c\nabla \cdot \xi$. In terms of the Green's function, we have

$$\Psi(r_j, \omega) = \int_V G(r_j, r, \omega)s(r, \omega)\rho dr$$

where the source $s(r, \omega)$ is a realization of a random process.

Plan

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Modal Green's kernel

Decomposition on harmonic mode ℓ, the modal Green's kernel G_ℓ solves,

$$\mathcal{L}\, G_\ell(r,s) = \delta(r-s), \qquad \text{with} \quad \mathcal{L} := \left(-\partial_r^2 - \frac{\omega^2 + 2\,\mathrm{i}\omega\,\Gamma}{c^2} + \frac{\alpha^2}{4} + \frac{\alpha'}{2} + \frac{\alpha}{r} + \frac{\ell(\ell+1)}{r^2} \right).$$

with Neumann boundary condition at origin: $\partial_n G_\ell(r=0) = 0,$
and radiation condition at $r = r_{\max}$: $(\partial_n G_\ell \; - \; \mathcal{Z}\, G_\ell)_{r=r_{\max}} = 0.$

H. Barucq, F. Faucher, H. Pham, Outgoing solutions and radiation boundary conditions for the ideal atmospheric scalar wave equation in helioseismology. ESAIM, 2020.

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Computation of the modal Green's kernel:

- **Approach 1 (naive)**: for each source position s, solving equation $\mathcal{L}\, G_\ell(r,s) \,=\, \delta(r-s)$ gives $G_\ell(\cdot, s)$.
- **Approach 2**: Use an assembling formula, the entire kernel is obtained from the solutions of only two boundary-value problems.

H. Barucq, F. Faucher, D. Fournier, L. Gizon and H. Pham, Efficient and accurate algorithm for the full modal Green's kernel of the scalar wave equation in helioseismology. SIAM J. on Appl. Math., 2020.

Computation of the Green's kernel: Approach 2

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- **Approach 2**: Use an assembling formula, the entire kernel is obtained from the solutions of only two boundary-value problems.

1. Find ψ_1 that solves
$$\begin{cases} \mathcal{L}\,\psi_1 = 0\,, & \text{on } (0, r_{\text{max}}), \\ (\partial_n \psi_1)_{r=0} = 0, & (\psi_1)_{r=r_b} = 1\,. \end{cases}$$

2. Find ψ_2 that solves
$$\begin{cases} \mathcal{L}\,\psi_2 = 0\,, & \text{on } (r_a, r_{\text{max}}), \\ (\psi_2)_{r=r_a} = 1, & (\partial_n \psi_2 - \mathcal{Z}\psi_2)_{r=r_{\text{max}}} = 0\,. \end{cases}$$

H. Barucq, F. Faucher, D. Fournier, L. Gizon and H. Pham, Efficient and accurate algorithm for the full modal Green's kernel of the scalar wave equation in helioseismology. SIAM J. on Appl. Math., 2020.

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3. Assemble the Green's kernel, with H the Heaviside and $\mathcal{W}$ the Wronskian $\mathcal{W}(s) := \mathcal{W}\{\psi_1(s), \psi_2(s)\}$,

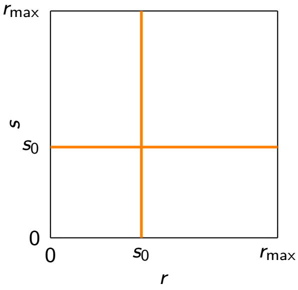
$$\boxed{G_\ell(r,s) = \frac{-H(s-r)\,\psi_1(r)\,\psi_2(s) \;-\; H(r-s)\,\psi_1(s)\,\psi_2(r)}{\mathcal{W}(s)}, \qquad \forall\,(r,s) \in (r_a, r_{\max}),}$$

H. Barucq, F. Faucher, D. Fournier, L. Gizon and H. Pham, Efficient and accurate algorithm for the full modal Green's kernel of the scalar wave equation in helioseismology. SIAM J. on Appl. Math., 2020.

Computation of the Green's kernel: Approach 2

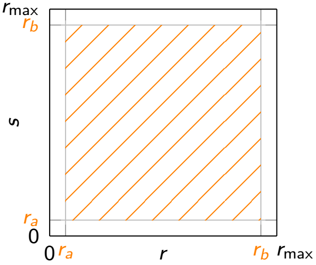
- **Approach 1 (naive)**: for each source position s, solve equation $\mathcal{L}\, G_\ell(r,s) = \delta(r-s)$.
- **Approach 2**: Use an assembling formula, the entire kernel is obtained from the solutions of only two boundary-value problems.

Approach 1: the solution of one problem for a Dirac in s_0 only gives $G_\ell(r, s = s_0)$ and $G_\ell(r = s_0, s)$.



Approach 2: from the solutions of two boundary value problems, $G_\ell(r,s)$ is obtained for any position between r_a and r_b.

It also avoids the singularity of the Dirac source.



Plan

6 Illustration: Green's function computations for time-distance helioseismology

- Modal Green's kernel
- Numerical experiments
- Power spectrum, comparison with measured data
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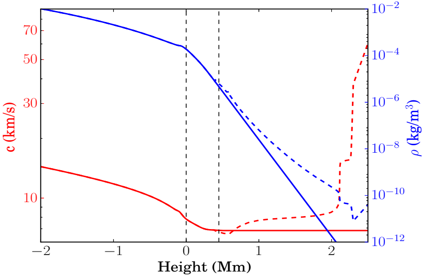
Solar Green's kernels

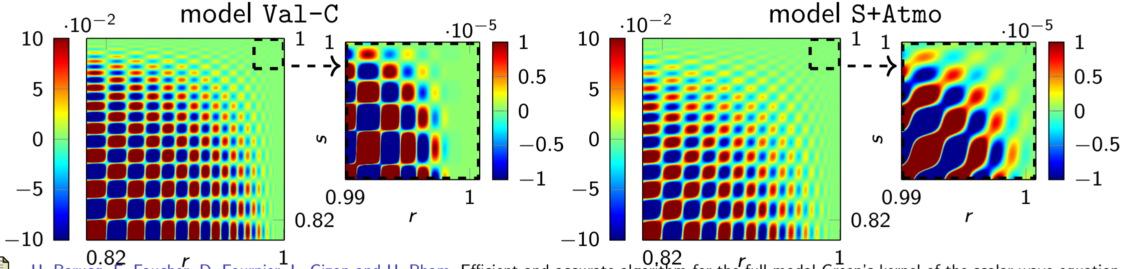
- The background sound-speed and density are given by `model S+Atmo` or `model Val-C`.



Solar Green's kernels

- The background sound-speed and density are given by `model S+Atmo` or model `Val-C`.
- The Green's kernel is computed with Approach 2 which only need the solutions of two problems.

Imaginary part of the Solar modal Green's functions at 7 mHz for mode $\ell = 100$ using different background.



H. Barucq, F. Faucher, D. Fournier, L. Gizon and H. Pham, Efficient and accurate algorithm for the full modal Green's kernel of the scalar wave equation in helioseismology. SIAM J. on Appl. Math., 2020

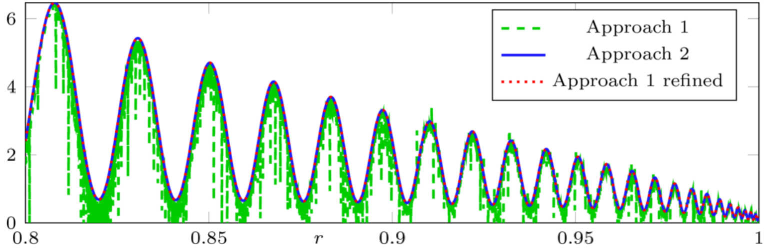
F. Faucher
hawen: time-harmonic wave modeling and inversion using hybridizable discontinuous Galerkin discretization
Journal of Open Source Software, 6 (57), 2021

Solar Green's kernels

- The background sound-speed and density are given by `model S+Atmo` or model `Val-C`.
- The Green's kernel is computed with Approach 2 which only needs the solutions of two problems.

Approach 2 is more **efficient** as it only needs two boundary value problems to assemble the entire kernel, and more **accurate** as it avoids the Dirac singularity.

1. To obtain $G_\ell(s, s)$ with Approach 1, we need 4000 simulations,
2. Approach 1 needs a refined discretization mesh to capture correctly the singularity.



Plan

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Power spectrum

Observables are an average over height of G_ℓ, in first approximation (depending on the assumption on the source), one can consider the Power Spectrum to be directly related to the Imaginary part of G_ℓ,

$$\mathcal{P}_\ell(\omega) \propto \Big| \mathrm{Im}\big(G_\ell(\omega)(r_0, s_0)\big) \Big|^2 . \tag{9}$$

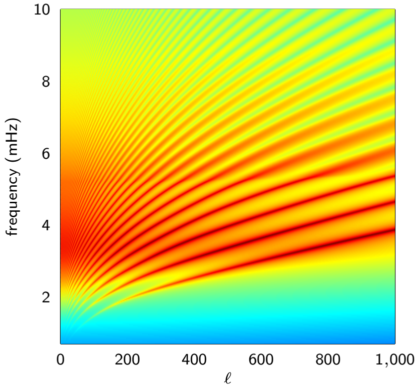
We can compare the numerical power spectrum, i.e., using Green's function computed for harmonic degrees (modes) ℓ and frequencies $\omega/(2\pi)$, with observations.

H. Barucq, F. Faucher, D. Fournier, L. Gizon and H. Pham, Efficient and accurate algorithm for the full modal Green's kernel of the scalar wave equation in helioseismology. SIAM J. on Appl. Math., 2020.

Power spectrum

We evaluate the imaginary part of the Green's function $G_\ell(r=1, s=1)$ with frequencies and modes, using `model S+Atmo`.

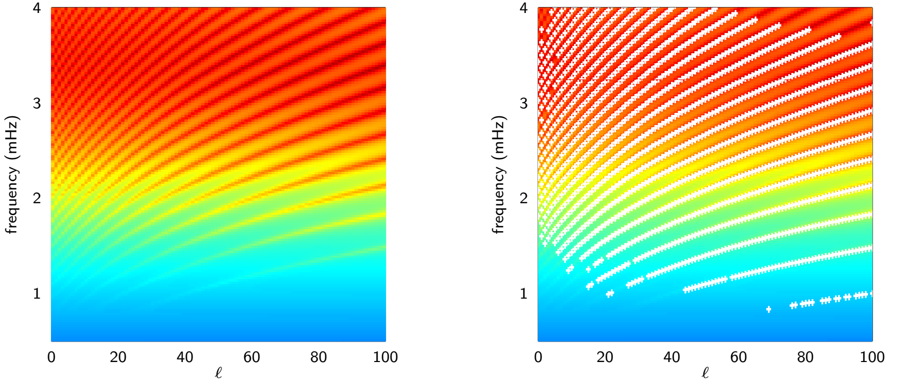
$$\ell \in (0,\ 1000), \qquad \omega/(2\pi) \in (0, 10)\text{mHz}.$$



Power spectrum

We evaluate the imaginary part of the Green's function $G_\ell(r = 1, s = 1)$ with frequencies and modes, using `model S+Atmo`.

Comparison with HMI data (white crosses), for $\ell \in (0, 100)$, $\omega/(2\pi) \in (0.5, 4)$mHz.



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Vector-wave equation with gravity

The same method can be applied to the vector-wave problem (Vector Spherical Harmonics),

$$-\rho_0\left(\omega^2+2\,\mathrm{i}\omega\,\Gamma\right)\,\xi-\nabla\left[\gamma\,p_0\nabla\cdot\xi\right]+(\nabla\,p_0)(\nabla\cdot\xi)-\nabla\,(\xi\cdot\nabla\,p_0)+(\xi\cdot\nabla)\nabla\,p_0+\rho_0\,(\xi\cdot\nabla)\nabla\,\phi_0\;=\;F\,,$$

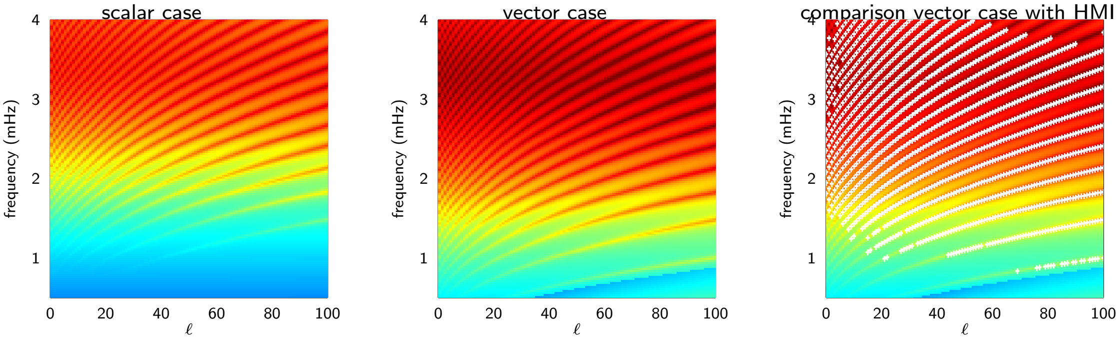
That is, the vector Green's kernels (depending on the direction) can be obtained from the computation of only two boundary-value problems.

H. Barucq, F. Faucher, D. Fournier, L. Gizon and H. Pham, Efficient computation of modal Green's kernels for vectorial equations in helioseismology under spherical symmetry. Research Report, 2021.

Vector-wave equation with gravity

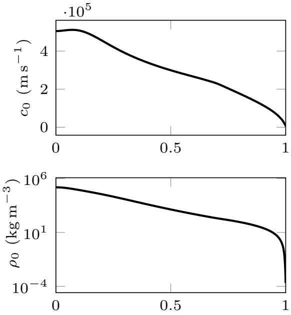
Comparison with HMI data (white crosses), for $\ell \in (0,\, 100)$, $\quad \omega/(2\pi) \in (0.5,\, 4)$mHz.

Including the gravity effect, f and g-modes now appear.

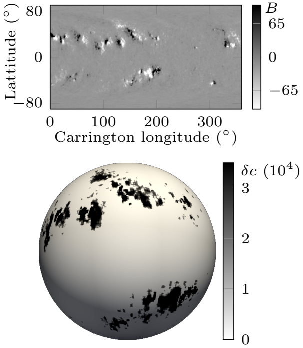


H. Barucq, F. Faucher, D. Fournier, L. Gizon and H. Pham, Efficient computation of modal Green's kernels for vectorial equations in helioseismology under spherical symmetry. Research Report, 2021.

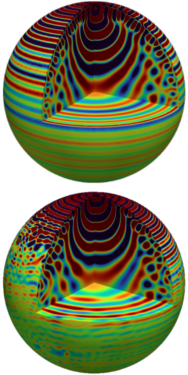
Towards 3D simulations



(a) spherical solar background models



(b) Active region as velocity perturbation



(c) Simulations with spherical background (top) and perturbations (bottom).

Scalar-wave propagation in global 3D Sun with in-house code hawen. The memory cost for its factorization is of 3 TiB.

Plan

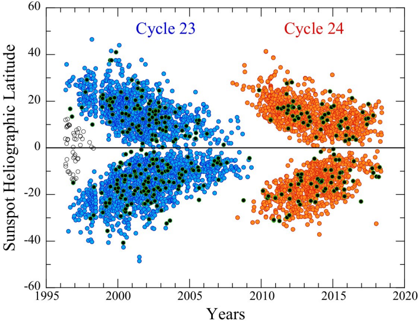
7 Conclusion

Recap

- Simulation of wave propagation provides a non invasive tool for probing the invisible
- Advanced numerical methods and HPC are mandatory
- Inversion remains very sensitive
- Recovering real data is also very sensitive and mathematical modeling has its part to play

Ongoing works

- Coupling SEM and DG for time-dependent problems in geophysics
- Conducting porous media
- Imaging 3D anisotropic elastic media with new acquisition methods (DAS)
- Solve the 3D Galbrun's equation with and without Cowling's approximation
- Construction of Butterfly diagrams for stars
- and so many very exciting problems



Makutu, September 2022

THANK YOU