The University of Queensland School of Earth and Environmental Sciences

Geophysical Modeling using esys-escript

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esys-escript

Geometry

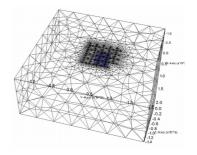
Mathematical Model

$$F = -A \nabla u - Bu + X$$

$$\nabla^{t} F + C \nabla u + Du = Y$$







esys-escript: scripted Model Implementation

from esys.escript import *
import esys.escript.unitsSI as U
Q=10^*U.W/U.m**3; K=1.7*U.W/(U.m*U.K); rhocp=1.5*U.Mega*U.J/(U.m**3*U.K)
#. __time_step_size: #. time step size:
dt=1."U.year; n_end=100
#...40 x 20 grid on 10km x 5km
mydomain=Rectangle(40, 20,10=10*U.km, 11=5*U.km)
x=mydomain=n_getX()
#...create PDE and set coefficients:
mydod=1.inearPDE (domain)
mydod. setValue(A=K*kronecker(mydomain), D=rhocp/dt, q=whereZero(x[1]-5*U.km)) # ... initial temperature is a vertical, linear profile: T=0*U.Celsius+30*U.K/U.km*(5*U.km.x[1]) n=0 while n<n_end : mule n<n_end :
mypde.setValue(Y=Q+rhocp/dt*T, r=T)
T=myPDE.getSolution()
n+=1

saveVTK("u%s"%n, temperature=T, flux=-K*grad(T))
print("Time ",n*dt,": min/max temperature =",inf(T), sup(T))





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Parallel Supercomputers







esys-escript (cont.)





• Modeling with PDEs $\rho c_p \frac{\partial T}{\partial t} - \nabla^t K \nabla T = Q$

$$\rho c_p \frac{\partial T}{\partial t} - \nabla^t K \nabla T = Q$$

Rapid prototyping of new models



Easy of Use



"Supercomputing for the masses"



- Open Source
- Programming in python python



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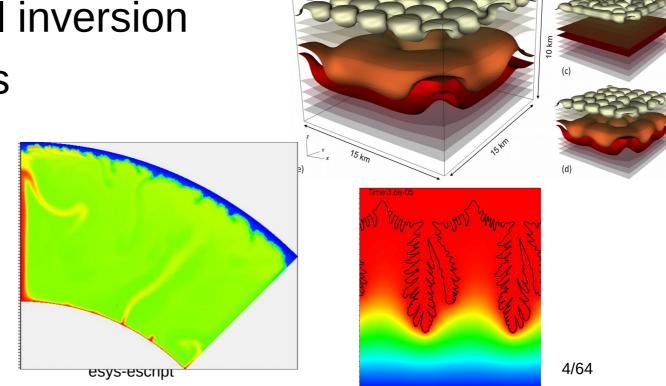
powered

Some applications

0.5000

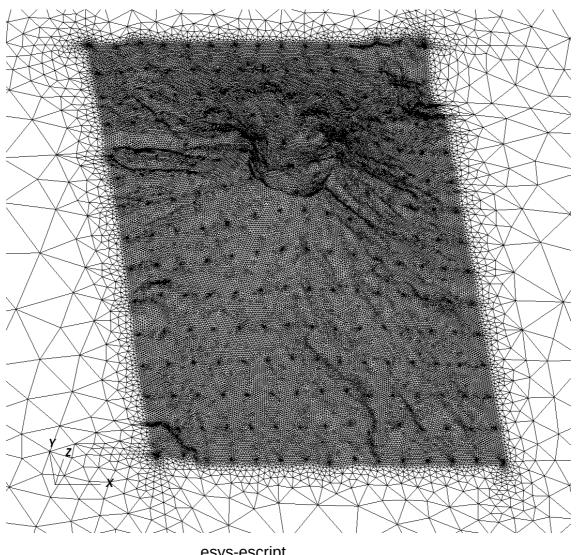
0.2500

- Mantel Convection
- Pores Media Flow
- Geomechanics
- Geophysical inversion
- Earthquakes
- Volcanoes
- Tsunamis
- •





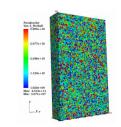
In 3D with topography





Discretization in esys-escript

- Finite Element Method (FEM)
 - Grids and unstructured meshes in 2D and 3D
- approximate solution PDEs in variational form
 - by continuous, piecewise linear approximation
 - Solve discrete problem with sparse matrix
 - With direct, iterative, multi-grid solver
- Parallelization on large number of cores (>25000)
 - Use Domain decomposition
 - Hidden from then user





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Downloads

- Program: https://launchpad.net/escript-finley
 - Installation from source
- API Documentation: https://esys-escript.readthedocs.io
- Anaconda: https://anaconda.org/conda-forge/esys-escript
- Flatpack store



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In this course

- Gravity Anomalies
- Magnetic Field
- Magnetotellurics
- Seismic Waves
 - in frequency domain
 - In time domain



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Python Script Structure

- (a) Definition of the domain
- (b) Definition of PDE coefficients
- (c) Obtain Solution
- (d) Post-processing
 - Get solution at points → recordings
 - ▶ Write to file → visualization



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Escript's PDEs

general linear PDE for unknown solution u:

'generalized' flux:
$$F = -A \nabla u + X$$

conservation equation:

$$\nabla^t \mathbf{F} + D u = \underbrace{Y}_{\text{volume source}} + \underbrace{y}_{\text{dirac}}$$



Escript's PDEs in 2D

$$\boldsymbol{F} = \begin{bmatrix} F_0 \\ F_1 \end{bmatrix} = - \begin{bmatrix} A_{00} \frac{\partial u}{\partial x_0} + A_{01} \frac{\partial u}{\partial x_1} + X_0 \\ A_{10} \frac{\partial u}{\partial x_0} + A_{11} \frac{\partial u}{\partial x_1} + X_1 \end{bmatrix} \qquad \boldsymbol{A} = \begin{bmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{bmatrix}$$

$$m{A} = egin{bmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{bmatrix}$$

$$\frac{\partial F_0}{\partial x_0} + \frac{\partial F_1}{\partial x_1} + Du = Y + y_{dirac}$$



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Escript's PDEs in Python

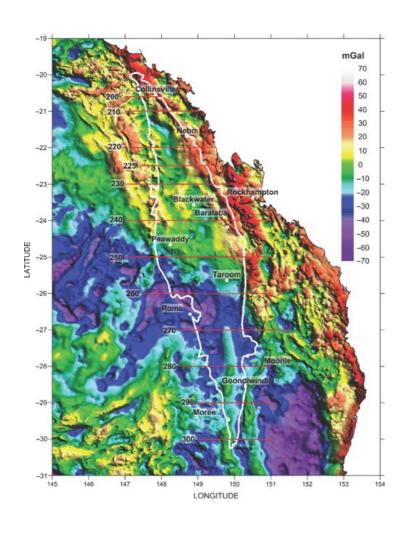
```
from esys.escript.linearPDEs import LinearSinglePDE
domain = ...
mypde=LinearSinglePDE(domain)
mypde.setValue(A=?, X=?, D=?, Y=?, y_dirac=?)
u=mypde.getSolution()
```

Identify PDE coefficients!?



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Modeling Gravity Anomaly

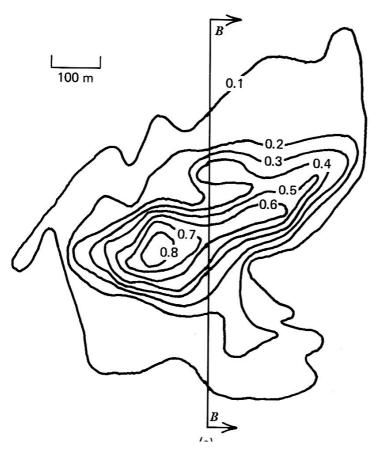




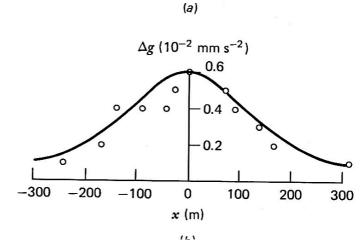
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Gravity Anomalies (cont.)

Contour plot of vertical gravity anomaly g₇



2D Interpolation of point observations



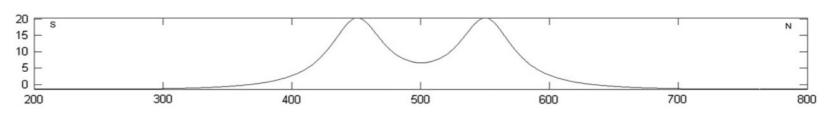




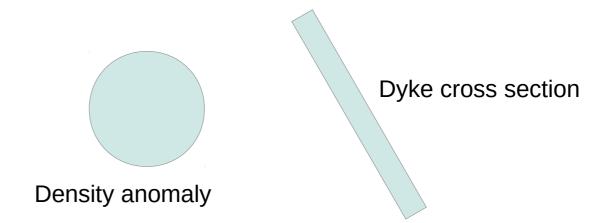
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Gravity anomaly

Deviation of g_z from background with constant density



Subsurface:





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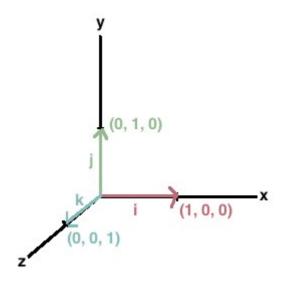
Gravity Force g as Vector Field

$$g = i g_x + j g_y + k g_z$$

unit vector x,y,z-direction : i, j, k

x,y,z components of $g:g_x,g_y,g_z$

$$g = (g_x, g_y, g_z)$$





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Gauss's law for gravity

Generalized version of Newton's law

$$\frac{\partial g_x}{\partial x} + \frac{\partial g_y}{\partial y} + \frac{\partial g_z}{\partial z} = -4 \pi G \rho$$

G=universal gravitational constant ρ =density (anomaly)



The Field Potential

- The gravity field ${\bf g}$ is expressed as the gradient of a the gravity potential ${\bf U}_{\rm G}$
 - Work with a scalar rather then vector quantity

$$\boldsymbol{g} = -\nabla U_G = -\left(\boldsymbol{i}\frac{\partial U_G}{\partial x} + \boldsymbol{j}\frac{\partial U_G}{\partial y} + \boldsymbol{k}\frac{\partial U_G}{\partial z}\right)$$

$$g_x = -\frac{\partial U_G}{\partial x}, g_y = -\frac{\partial U_G}{\partial y}, g_z = -\frac{\partial U_G}{\partial z}$$



Compact Form

$$g = -\nabla U_G$$

$$\nabla^t \cdot \boldsymbol{g} = -4 \pi G \rho$$

 ∇ = gradient operator

 ∇^t =divergence operator



In Escript?

$$\nabla^{t} \cdot \mathbf{g} = -4\pi G \rho \qquad \qquad \nabla^{t} \mathbf{F} + D u = \mathbf{Y} + \mathbf{y}_{dirac}$$

$$\mathbf{g} = \mathbf{F} \qquad \begin{aligned} \mathbf{Y} &= -4\pi G \rho \\ \mathbf{y}_{dirac} &= 0 \quad D = 0 \end{aligned}$$

$$U_{G} = u \quad \mathbf{A} = \mathbf{I} \\ \mathbf{X} &= \mathbf{0}$$

 $q = -\nabla U_G$ $F = -A \nabla u + X$



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Escript's PDEs in 2D

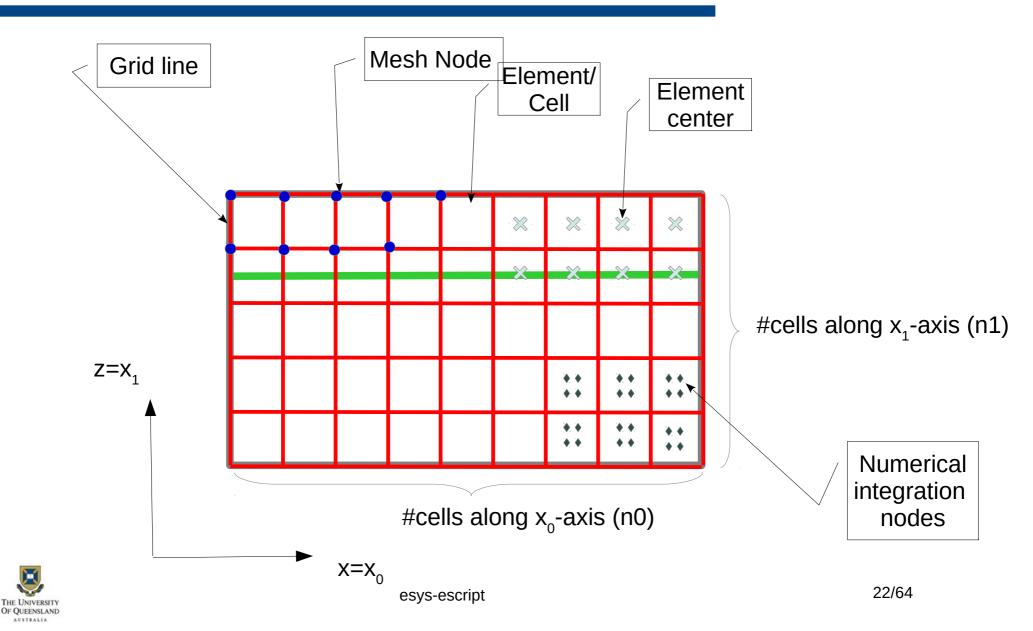
$$u=U_G, x_0=y, x_1=z$$

$$\boldsymbol{F} = \begin{bmatrix} F_0 \\ F_0 \end{bmatrix} = \begin{bmatrix} g_y \\ g_z \end{bmatrix} = - \begin{bmatrix} A_{00} \frac{\partial u}{\partial x_0} + A_{01} \frac{\partial u}{\partial x_1} \\ A_{10} \frac{\partial u}{\partial x_0} + A_{11} \frac{\partial u}{\partial x_1} \end{bmatrix} = - \begin{bmatrix} \frac{\partial u}{\partial x_0} \\ \frac{\partial u}{\partial x_1} \end{bmatrix} \qquad \boldsymbol{A} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\frac{\partial F_0}{\partial x_0} + \frac{\partial F_1}{\partial x_1} = \frac{\partial g_y}{\partial x_1} + \frac{\partial g_z}{\partial x_1} = Y = -4\pi G\rho$$



Grid/Mesh Representation



Grids/meshes

- Terminology: n0 x n1 grid
 - Example before: 9x5 grid
- Quantities are represented by values
 - At Nodes or
 - At Cell centers or
 - At Integration nodes



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Mesh/Grid Generation

 Here we use 2D rectangular Domain with a rectangular grid:

```
from esys.finley import Rectangle dx=10
```

n0, n1=100, 100

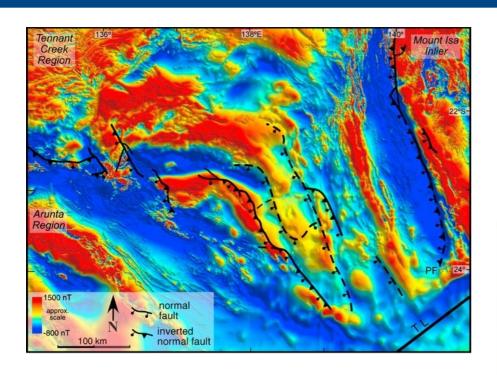
Lx=Nx*dx

Ly=Ny*dx

domain=Rectangle(n0=Nx, n1=Ny, l0=Lx, l1=Ly)

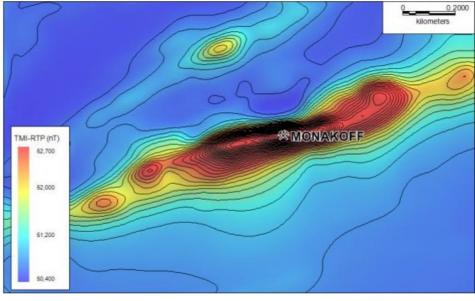


Magnetic Anomaly Mapping



Here: magnetic field anomaly

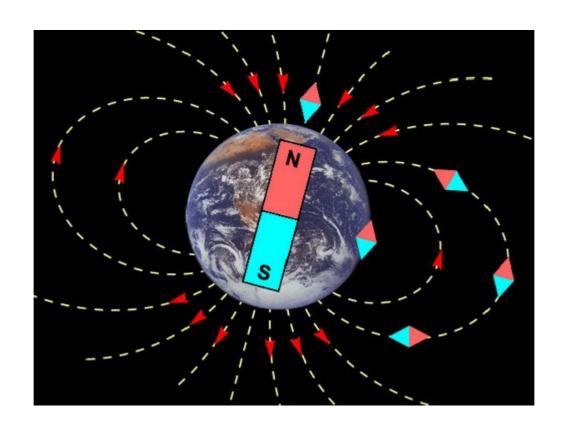
=
difference of total and background field
intensity





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Background Magnetic Field





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Magnetic Field

Magnetic Induction B_I is sum of magnetic field
 B_t and magnetization M:

$$\boldsymbol{B}_{I} = \boldsymbol{M} + \boldsymbol{B}_{t}$$

Magnetic Induction is divergence free:

$$\nabla^t \mathbf{B}_I = 0$$



Susceptibility

Magnetization \mathbf{M} is proportional to background magnetic field \mathbf{B}_h

$$M = k B_b$$

- With susceptibility k,
 - -0 < k < 1
 - Causes magnetic anomalies
 - Is depending on location in the subsurface



The Field Potential

- The magnetic field ${\bf B}$ is expressed as the gradient of a the gravity potential ${\bf U}_{\rm M}$
 - Work with a scalar rather then vector quantity

$$\boldsymbol{B} = -\nabla U_{M} = -\left(i\frac{\partial U_{M}}{\partial x} + j\frac{\partial U_{M}}{\partial y} + k\frac{\partial U_{M}}{\partial z}\right)$$

$$B_x = -\frac{\partial U_G}{\partial x}, B_y = -\frac{\partial U_G}{\partial y}, B_z = -\frac{\partial U_G}{\partial z}$$



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Governing Equation

set:
$$\mathbf{B} = \mathbf{B_t} - \mathbf{B_h}$$
 assume: $\nabla^t \mathbf{B_b} = 0$

$$\nabla^{t}(k\mathbf{B}_{h}+\mathbf{B})=0$$

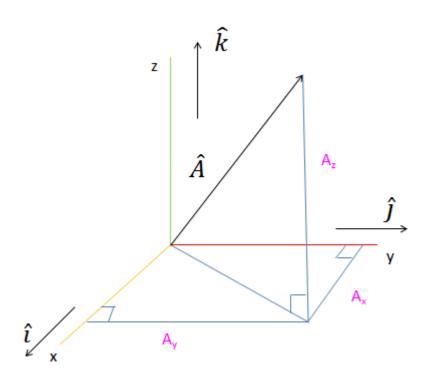
$$\mathbf{B}=-\nabla U_{M}$$



Intensity of a Field

Intensity, length, norm:

$$b = |\mathbf{B}| = \sqrt{B_x^2 + B_y^2 + B_z^2}$$





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Magnetic Field Anomaly

=Difference of the intensity of the total magnetic field \mathbf{B}_{t} and the intensity of the background magnetic field \mathbf{B}_{b}

$$b_a = |\boldsymbol{B_t}| - |\boldsymbol{B_b}|$$

$$\boldsymbol{B}_{t} = \boldsymbol{B} + \boldsymbol{B}_{b}$$



Modeling magnetic response?

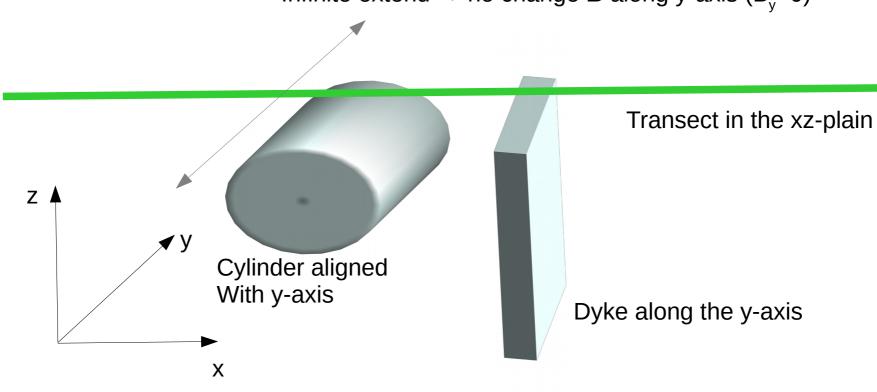
- Given an anomaly in the subsurface as
 - Susceptibility distribution/anomaly k
 - Background magnetic field B_H
- What is the total total magnetic field anomaly in the subsurface?



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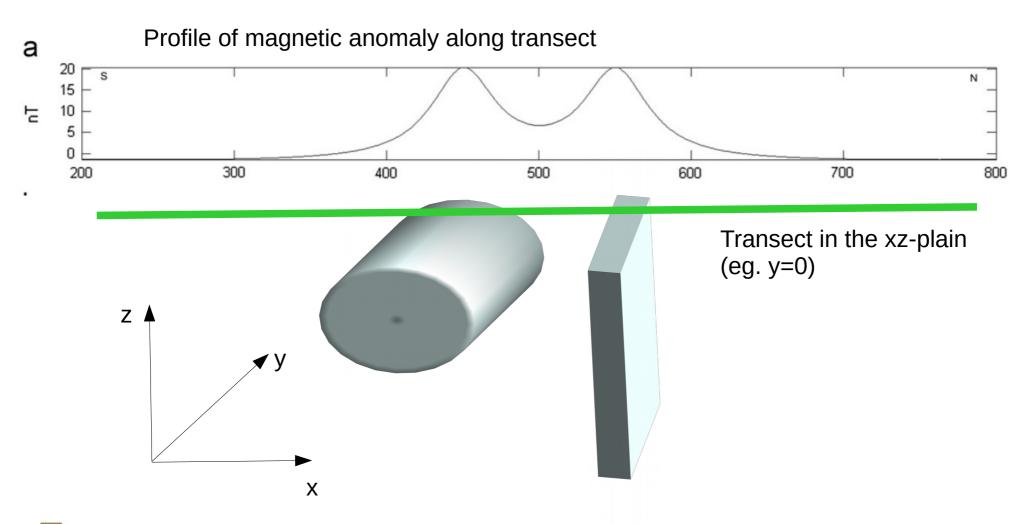
2D Modeling Setup

Infinite extend \rightarrow no change **B** along y-axis (B_v=0)





2D Modeling Setup





In Escript?

$$\nabla^{t}(k \mathbf{B}_{h} + \mathbf{B}) = 0 \qquad \nabla^{t} \mathbf{F} + D u = Y + y_{dirac}$$

$$\mathbf{B} + k \mathbf{B}_{h} = \mathbf{F} \qquad D = 0$$

$$y_{dirac} = 0$$

$$Y_{dirac} = 0$$

$$\mathbf{A} = \mathbf{I}$$

$$\mathbf{X} = k \mathbf{B}_{h}$$

$$\mathbf{F} = -\nabla U_{M} + k \mathbf{B}_{h} \qquad \mathbf{F} = -\mathbf{A} \nabla u + \mathbf{X}$$



Escript's PDEs in 2D

$$u=U_M, x_0=y, x_1=z$$

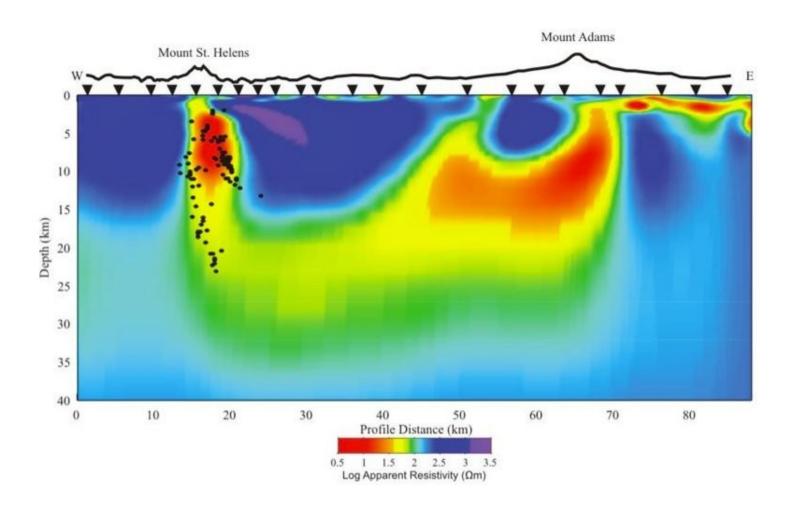
$$\boldsymbol{F} = \begin{bmatrix} F_0 \\ F_1 \end{bmatrix} = \begin{bmatrix} B_y + k B_{by} \\ B_z + k B_{bz} \end{bmatrix} = -\begin{bmatrix} \frac{\partial u}{\partial x_0} + X_0 \\ \frac{\partial u}{\partial x_1} + X_1 \end{bmatrix} = -\begin{bmatrix} A_{00} \frac{\partial u}{\partial x_0} + A_{01} \frac{\partial u}{\partial x_0} + X_0 \\ A_{10} \frac{\partial u}{\partial x_0} + A_{11} \frac{\partial u}{\partial x_1} + X_1 \end{bmatrix}$$

$$\begin{bmatrix} X_0 \\ X_1 \end{bmatrix} = \begin{bmatrix} k B_{by} \\ k B_{bz} \end{bmatrix} \quad \mathbf{A} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\frac{\partial F_0}{\partial x_0} + \frac{\partial F_1}{\partial x_1} = \frac{\partial}{\partial x_1} (B_y + k B_{by}) + \frac{\partial}{\partial x_1} (B_z + k B_{bz}) = Y = 0$$



Magnetotellurics (MT)





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The Method of Magnetotellurics

- passive electromagnetic (EM) method
 - Target: subsurface resistivity distribution
- naturally generated source field by variations in

Earth's magnetic field

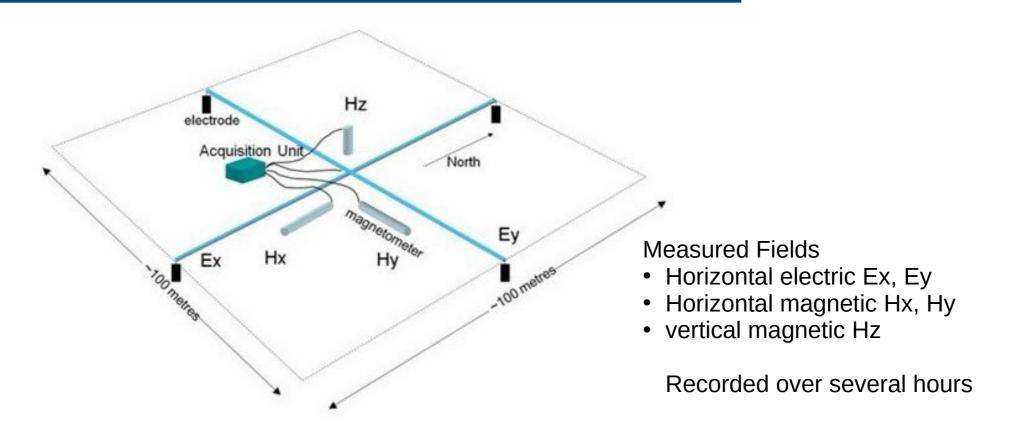
- EM field from the sum (<1Hz)
- Lightnings (>1Hz)





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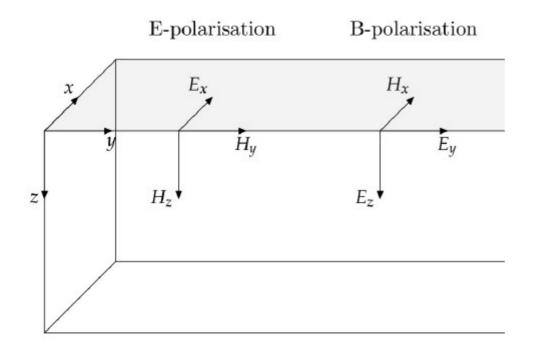
Survey Design





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TM-mode: H-Polarisation



Measurements provide Impedance defined as

$$Z_{yx} = \frac{E_y}{H_x}$$

Depending of frequency f of incoming wave!



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Quantities For Interpretation

• Apparent Resistivity for angular frequency $\omega = 2\pi f$

$$\rho_a = \frac{1}{\omega \mu_0} |Z_{yx}(\omega)|^2$$

Phase of impedance:

$$\phi = \arctan(\frac{Z_{yx}(\omega).imag}{Z_{yx}(\omega).real})$$

$$\mu_0 = 1.26 \cdot 10^{-6} \frac{mkg}{s^2 A^2}$$

- ullet To obtain information on subsurface conductivity σ
 - look at dependency on ω
 - Use 2D or 3D profiles at surface



Modeling equations: TM mode

$$\frac{\partial H_{x}}{\partial y} = -\sigma E_{z}$$

$$\frac{\partial H_{x}}{\partial z} = \sigma E_{y}$$

$$\frac{\partial E_{z}}{\partial y} - \frac{\partial E_{y}}{\partial z} = -\mathbf{j} \omega \mu_{0} H_{x}$$



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Recall Esys-escript PDE template

flux:
$$\mathbf{F} - \mathbf{A} \nabla u + \mathbf{X} = \begin{bmatrix} -A_{00} \frac{\partial u}{\partial x_0} - A_{01} \frac{\partial u}{\partial x_0} - X_0 \\ -A_{10} \frac{\partial u}{\partial x_0} - A_{11} \frac{\partial u}{\partial x_1} - X_1 \end{bmatrix}$$

conservation equation:

$$Y = \nabla^{t} \mathbf{F} + D u = \frac{\partial F_{0}}{\partial x_{0}} + \frac{\partial F_{1}}{\partial x_{1}} + D u$$



TM in esys.escript (cont.)

conservation equation:

$$Y = \frac{\partial F_0}{\partial x_0} + \frac{\partial F_1}{\partial x_1} + Du$$

$$Y = \frac{\partial F_0}{\partial x_0} + \frac{\partial F_1}{\partial x_1} + Du \qquad \frac{\partial E_z}{\partial y} - \frac{\partial E_y}{\partial z} = -\mathbf{j} \omega \mu_0 H_x$$

flux:
$$\mathbf{F} = \begin{bmatrix} F_0 \\ F_1 \end{bmatrix} = \begin{bmatrix} E_z \\ -E_y \end{bmatrix}$$

$$D = \boldsymbol{j} \omega \mu_0 \quad Y = 0$$



TM in esys.escript (cont.)

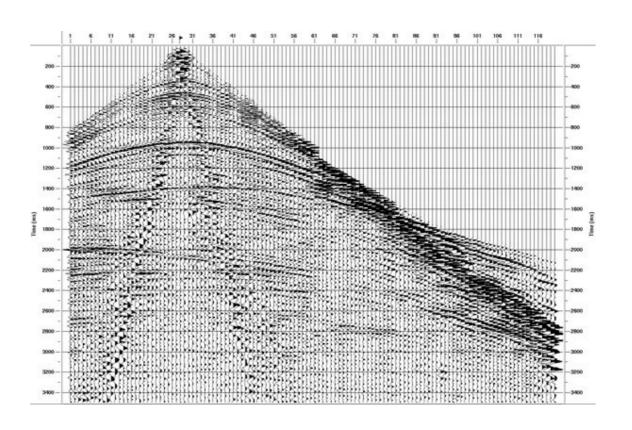
$$\frac{\partial H_{x}}{\partial y} = -\sigma E_{z} \qquad \frac{\partial H_{x}}{\partial z} = \sigma E_{y}$$

$$\mathbf{F} = \begin{bmatrix} E_{z} \\ -E_{y} \end{bmatrix} = \begin{bmatrix} -\frac{1}{\sigma} \frac{\partial H_{x}}{\partial y} \\ -\frac{1}{\sigma} \frac{\partial H_{x}}{\partial z} \end{bmatrix} = -\begin{bmatrix} \frac{1}{\sigma} \frac{\partial u}{\partial x_{0}} + 0 \frac{\partial u}{\partial x_{1}} \\ 0 \frac{\partial u}{\partial x_{0}} + \frac{1}{\sigma} \frac{\partial u}{\partial x_{1}} \end{bmatrix}$$

$$u = H_{x} \qquad X = 0 \qquad A = \begin{vmatrix} \frac{1}{\sigma} & 0 \\ 0 & \frac{1}{\sigma} \end{vmatrix}$$



Wave propagation

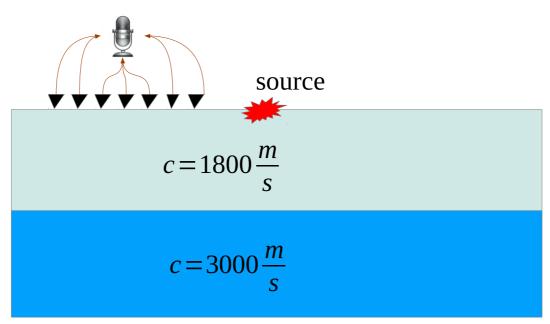




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Synthetic seismograms







Wave Propagation model

Sonic wave equation in time domain

$$\frac{1}{\rho c^2} \frac{\partial^2 p}{\partial t^2} = \nabla^t \frac{1}{\rho} \nabla p + \dot{w}(t) \cdot \delta_{x_s}$$

- w(t) source wavelet
- Point source @ x_s by Dirac δ-Function
- p(x,t) pressure function of t and x
- Density ρ
- p-wave propagation speed

$$c = v_p = \sqrt{\frac{K + \frac{4}{3}G}{\rho}}$$



In Frequency Domain

Apply Fourier Transformation on time:

$$\hat{p}(\mathbf{x},\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} p(\mathbf{x},t) e^{i\omega t} dt$$

- Angular frequency ω
- \hat{p} is complex!
- As p is real: $\hat{p}(x,\omega) = \hat{p}(x,-\omega)$
 - We need to look at ω≥0 only.



Wave Equation in Frequency Domain

$$-\nabla^{t}\nabla p - k^{2}p = P_{s\omega} \cdot \delta_{x_{s}}$$

$$k = \frac{\omega}{c}$$

- Solution p=p(x;ω,s)
- $P_{s\omega}$ power amplitude for point source at \mathbf{x}_s
- Assume constant density



Solution rescaling

$$-\nabla^t \nabla u - k^2 u = \delta_{x_s}$$

$$p(x;\omega,s)=P_{\omega s}\cdot u(x;\omega,s)$$

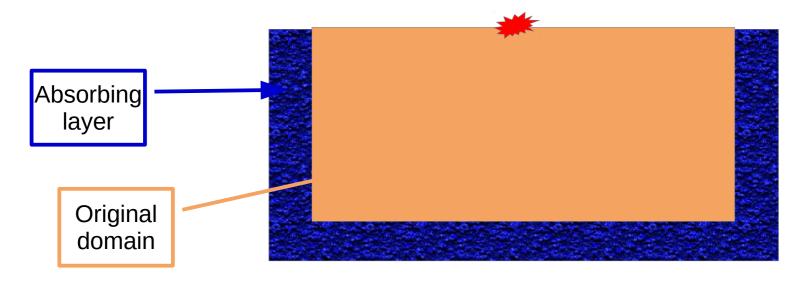
$$-\frac{\partial^2 u}{\partial x_0^2} - \frac{\partial^2 u}{\partial x_1^2} + k^2 u = \delta_{x_s}$$



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Boundary Reflection

- Undesirable wave front reflected from numerical domain boundary
- Introduce wave absorbing layer near boundary
 - → Perfect Matching Layers (PML)





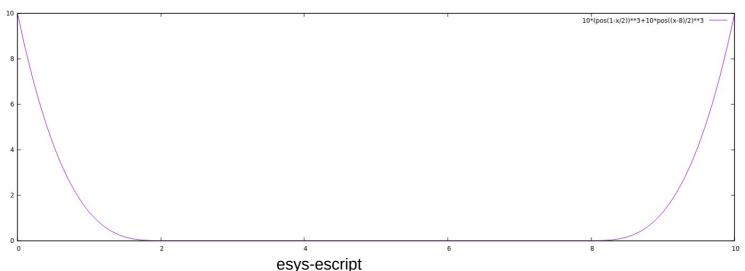
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Perfect Matching Layers (PML)

coordinate trafo:
$$x_i \rightarrow y_i \cdot x_i$$

$$\gamma_i = \left(1 - \mathbf{j} \frac{S}{k} Q_i\right)$$

 $Q_i(x_i)=1$ near the boundries $x_i=0$; $x_i=L_i$





PML (cont.)

$$-\frac{1}{\gamma_0}\frac{\partial}{\partial x_0}\frac{1}{\gamma_0}\frac{\partial u}{\partial x_0} - \frac{1}{\gamma_1}\frac{\partial}{\partial x_1}\frac{1}{\gamma_1}\frac{\partial u}{\partial x_1} - k^2u = \delta_{x_s}$$

multiply by: $\gamma_0 \gamma_1$, use γ_i depends on x_i only!

$$-\frac{\partial}{\partial x_0} \frac{\gamma_1}{\gamma_0} \frac{\partial u}{\partial x_0} - \frac{\partial}{\partial x_1} \frac{\gamma_0}{\gamma_1} \frac{\partial u}{\partial x_1} - k^2 \gamma_0 \gamma_1 u = \delta_{x_s}$$



In Esys-escript PDE template

conservation equation:

$$y_{dirac} + Y = \frac{\partial F_0}{\partial x_0} + \frac{\partial F_1}{\partial x_1} + Du$$

flux:
$$\mathbf{F} = \begin{bmatrix} -\frac{y_1}{y_0} \frac{\partial u}{\partial x_0} \\ -\frac{y_1}{y_0} \frac{\partial u}{\partial x_0} \end{bmatrix}$$

$$D = -k^{2} \gamma_{0} \gamma_{1}$$

$$y_{dirac} = \delta_{x_{s}}$$

$$Y = 0$$

$$-\frac{\partial}{\partial x_0} \frac{\gamma_1}{\gamma_0} \frac{\partial u}{\partial x_0} - \frac{\partial}{\partial x_1} \frac{\gamma_0}{\gamma_1} \frac{\partial u}{\partial x_1} - k^2 \gamma_0 \gamma_1 u = \delta_{x_s}$$



Recall Esys-escript PDE template

$$\mathbf{F} = \begin{bmatrix} -\frac{\gamma_1}{\gamma_0} \frac{\partial u}{\partial x_0} \\ -\frac{\gamma_1}{\gamma_0} \frac{\partial u}{\partial x_0} \end{bmatrix} = \begin{bmatrix} -A_{00} \frac{\partial u}{\partial x_0} - A_{01} \frac{\partial u}{\partial x_0} - X_0 \\ -A_{10} \frac{\partial u}{\partial x_0} - A_{11} \frac{\partial u}{\partial x_1} - X_1 \end{bmatrix}$$

$$\boldsymbol{X} = \begin{bmatrix} \frac{\mathbf{y}_1}{\mathbf{y}_0} & 0 \\ 0 & \frac{\mathbf{y}_0}{\mathbf{y}_1} \end{bmatrix}$$



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Wave Equation in Time Domain

$$\frac{1}{\rho c^2} \frac{\partial^2 p}{\partial t^2} = \nabla^t \frac{1}{\rho} \nabla p + \dot{w}(t) \cdot \delta_{x_s}$$

esys-escript



Wave Equation in Time Domain

$$\frac{1}{\rho c^2} \ddot{p} = \nabla^t \frac{1}{\rho} \nabla p + \dot{w}(t) \cdot \delta_{x_s}$$

Translate to system of first order problems:

$$\dot{\mathbf{V}} = \frac{1}{\rho} \nabla p$$

$$\frac{1}{\rho c^2} \dot{p} = \nabla^t V + w(t) \cdot \delta_{x_s}$$



Time Integration

Heun scheme solving :

$$\dot{U} = f(U,t)$$
for $U^{(n)} = U(t^{(n)})$ with $t^{(n)} + n \cdot h$

$$\hat{U}^{(n+1)} = U^{(n)} + h f(U^{(n)}, t^{(n)})$$

$$\bar{U}^{(n+1)} = \hat{U}^{(n+1)} + h f(\hat{U}^{(n+1)}, t^{(n+1)})$$

$$U^{(n+1)} = \frac{1}{2} (U^{(n)} + \bar{U}^{(n+1)})$$

$$n \leftarrow n + 1$$



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Application to Wave

$$U = \begin{bmatrix} V \\ p \end{bmatrix}$$

$$\boldsymbol{U} = \begin{bmatrix} \boldsymbol{V} \\ p \end{bmatrix} \qquad f(\boldsymbol{U}, t) = \begin{bmatrix} \boldsymbol{V}' \\ p' \end{bmatrix}$$

With

$$\mathbf{V}' = \frac{1}{\rho} \mathbf{\nabla} p$$

$$\frac{1}{\rho c^{2}} p' = \mathbf{\nabla}^{t} \mathbf{V} + w(t) \cdot \delta_{x_{s}}$$



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Solve PDE for u=p'

$$\frac{1}{\rho c^2} p' = \nabla^t \mathbf{V} + w(t) \cdot \delta_{\mathbf{x}_s}$$

$$F = -A \nabla u + X = -V$$

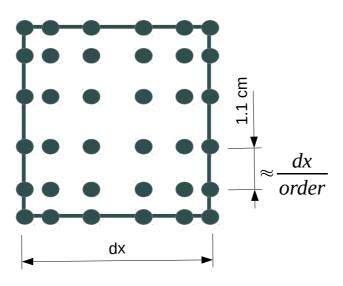


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Spectral Element Method (SEM)

- Implemented in the esys.speckley module
- Higher polynomial order polynomial
 - Non-equidistant nodes
 - Very good for waves

A grid cell:





Stability & Accuracy

- Small step size for stability:
 - In a time step wave travels never more than a node spacing:

$$h < \frac{dx}{order} \cdot \frac{1}{max_x c(x)}$$

- Small element size for accuracy:
 - Wave length is never shorter than the node spacing:

$$dx < \frac{order}{2\pi f_{max}} \cdot min_{x} c(x)$$

$$f_{max} \text{ maximum frequency in wavelet}$$

