Developer School
for HPC applications in Earth Sciences
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An Introduction
To Numerical Modelling in Seismology

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seismological processes in the Earth

(normal) tectonic earthquake

- long-term preparation of an earthquake
- spontaneous rupture initiation
- spontaneous rupture propagation
- generation of seismic waves
- propagation of seismic waves
- earthquake motion at the Earth‘s free surface
- earthquake ground motion in local surface structures (sedimentary bodies, topographic features)

body waves	(P and S)	0.01	–	50 sec
surface waves	(Love and Rayleigh)	10	–	350 sec

slow to silent earthquakes

artificially generated seismic waves in seismic exploration

$\sim$ 1 – 1000 Hz, typical frequency: $\sim$ 100 Hz

- explosive sources
- vibratory sources (vibroseis system)

both types of source

produce primarily P waves

seismic noise – continuous mechanical vibration of the ground

(typical amplitudes 0.1 to 10 μm/s)

natural sources ; <≅ 1 Hz

- ocean waves; 0.1-0.3 Hz
- variations of atmospheric pressure
- wind
- water flows
- magma movements
- ...

man-made sources ; > 1 Hz

- transportation (undeground, surface, air)
- mechanical machines
- all kinds of vibratory machinery
- ...

non-volcanic tremors – unusual tectonic seismic events

- long durations

  (from several minutes to hours)

- low amplitudes
- lack of P- and S- wave arrivals
- frequency content

  (often studied between 1 and 15 Hz)

- deeper origin compared to regular earthquakes in the fault zones

Earth‘s free oscillations

generated by the largest earthquakes

350 – 3600 sec

nuclear explosions

produce primarily P waves

comparable in released energy with moderate earthquakes

seismological processes in the Earth

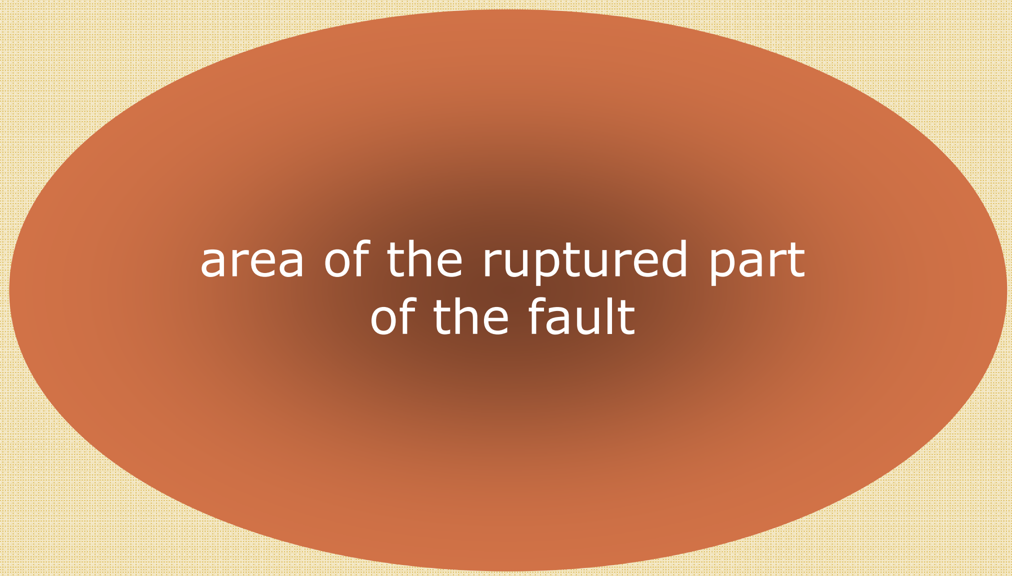
induced seismicity – small tectonic events

induced by / triggered by / due to

- water reservoir
- deep well
- fluid extraction
- mining
- volcanic eruption
- underground nuclear explosion
- tides

scalar seismic moment of tectonic events

fault



$$M_0 = \mu \cdot A \cdot D$$

$$\left[Nm = Nm^{-2} \cdot m^2 \cdot m \right]$$

μ torsion modulus

A ruptured area

D average slip

$\approx 10^{23}\ Nm$ Chile 1960

$\approx 10^{5}\ Nm$ microearthquake

$\approx 10^{-2}\ Nm$ microfracture in an laboratory sample

models of the Earth` interior

models

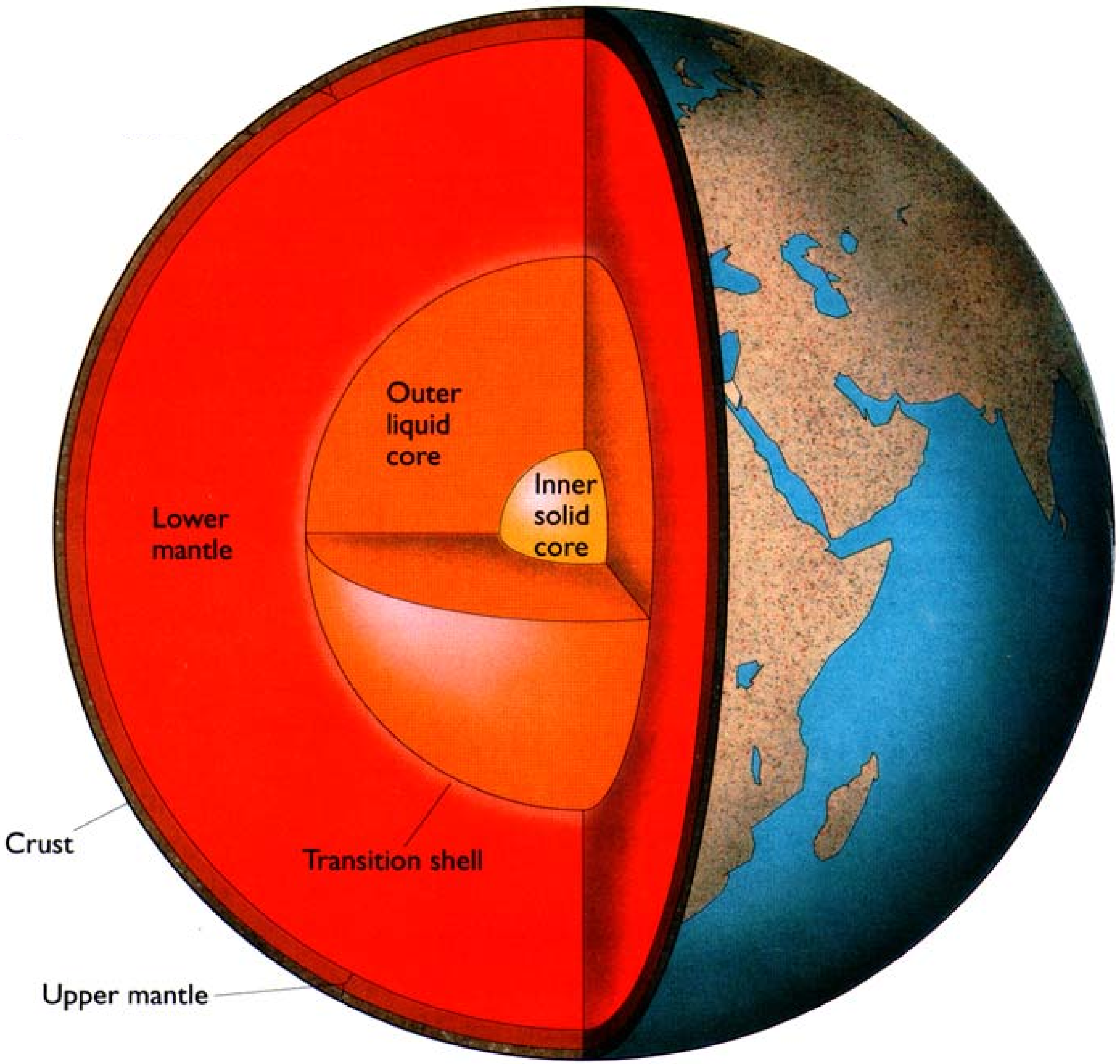
- geological
- physical
- discrete (grid)

physical model

spatial distribution of all material parameters
determining rupture and/or seismic wave propagation
for a considered rheological model

basic physical models of the Earth‘ interior

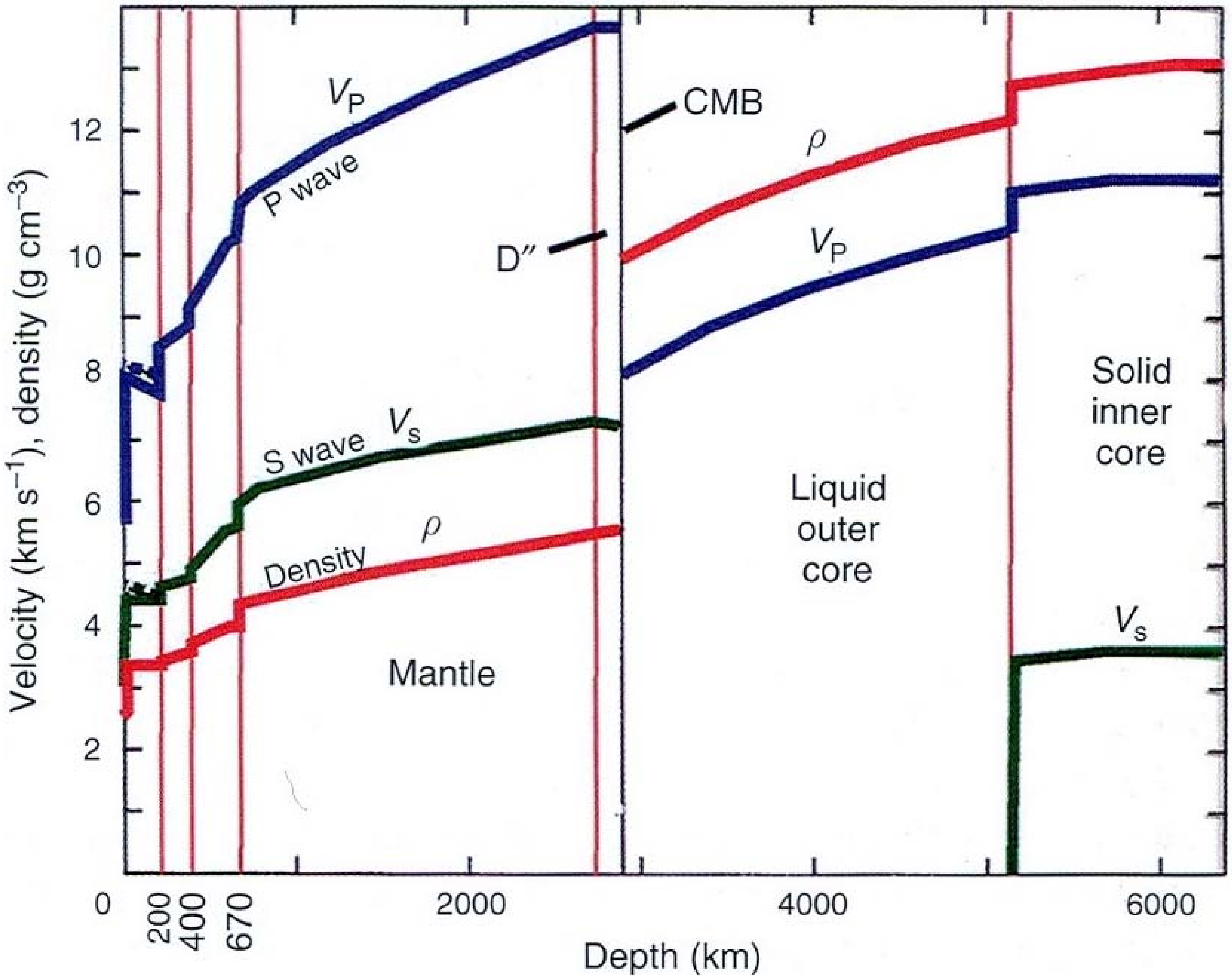
global spherically symmetric static (chemical) model

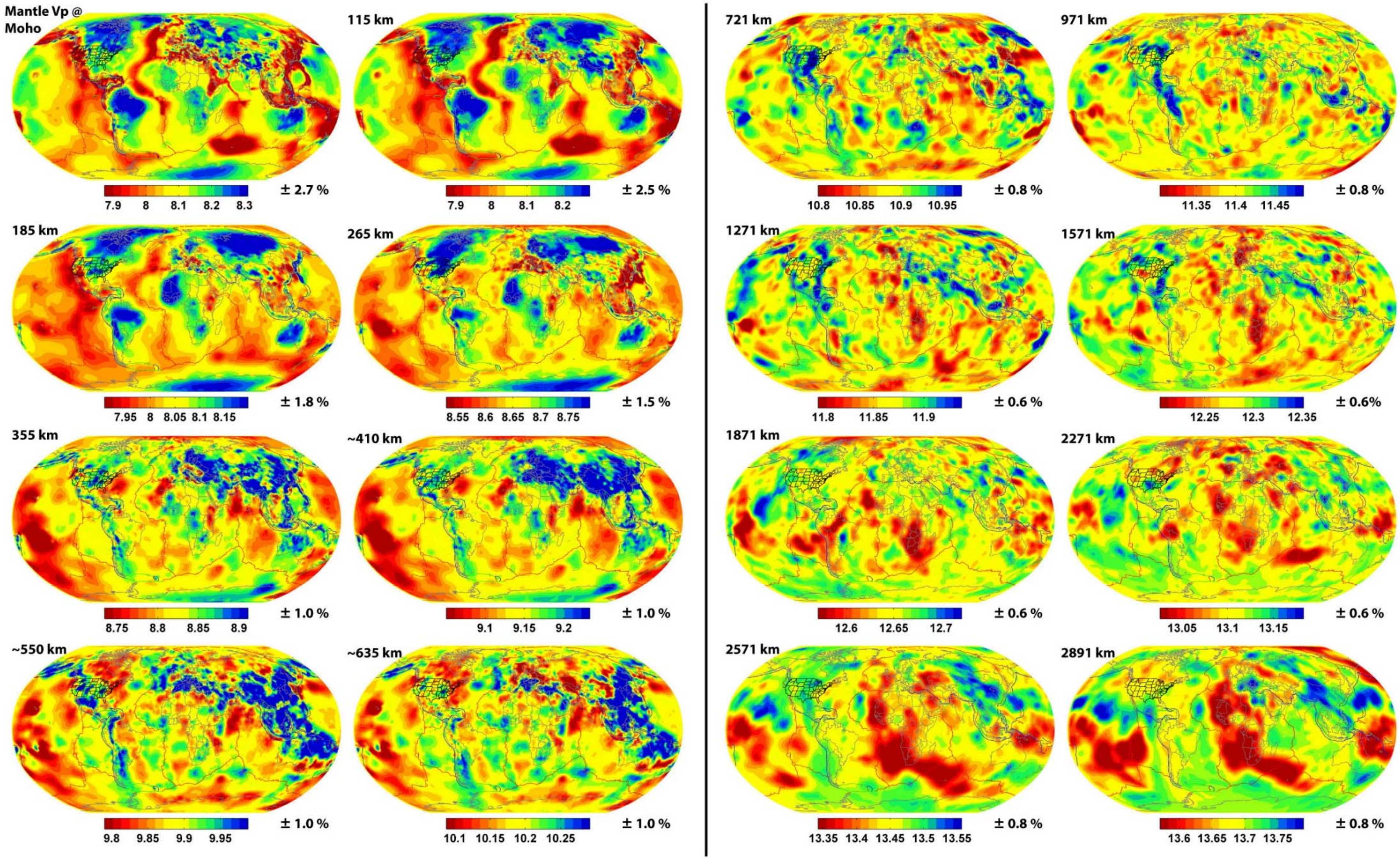


basic physical models of the Earth‛ interior

global spherically symmetric model:
P-wave and S-wave velocities, density
(Q factors not so well determined)

The Preliminary Reference Earth Model (PREM) of Dziewonski and Anderson (1981)





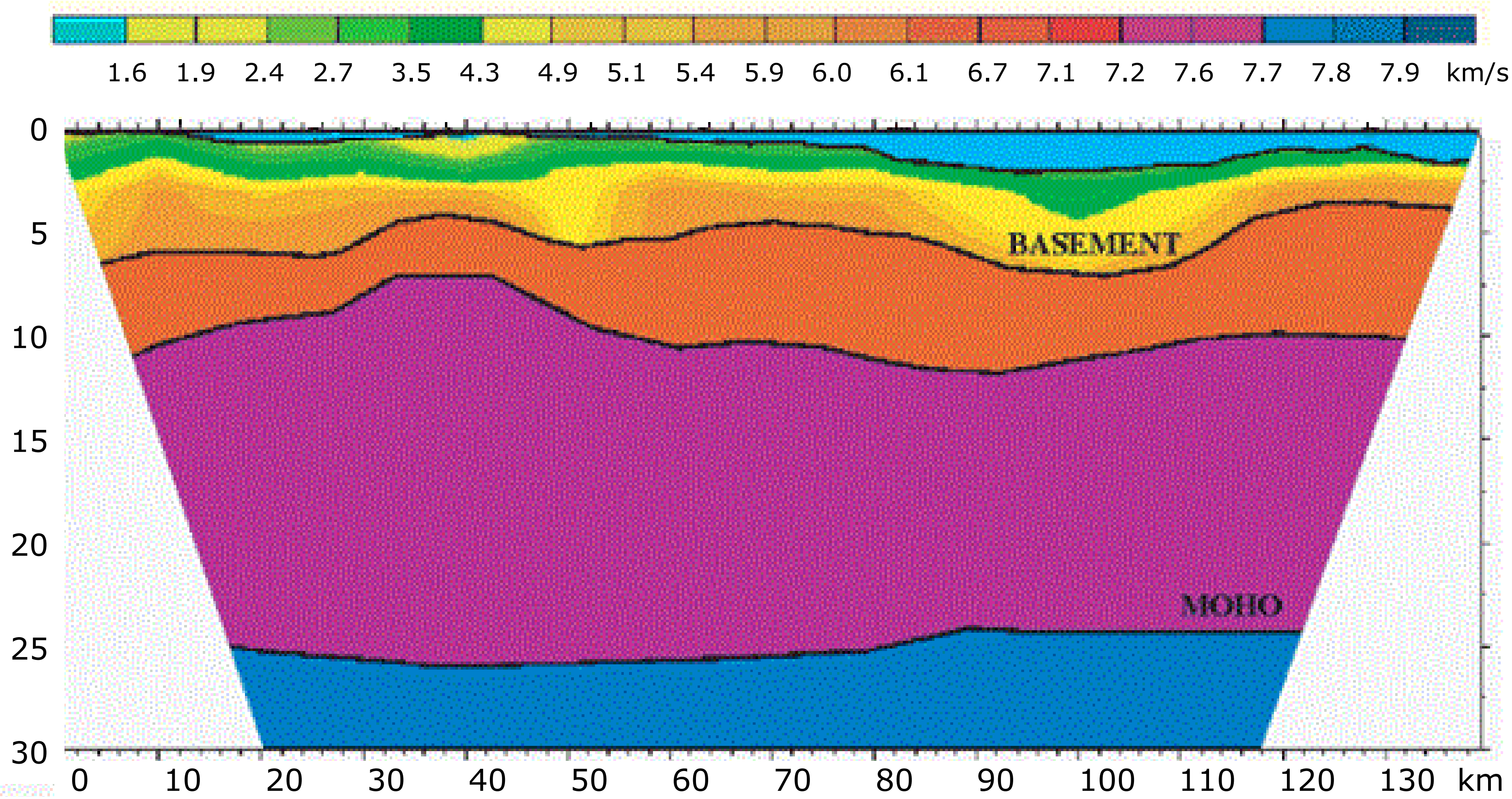
LLNL-G3Dv3 (Simmons et al. 2012)
a global-scale model of the crust and mantle P-wave velocity

basic physical models of the Earth' interior

regional velocity model down to depth of 30 km:

cross-section of the Kos-Yali-Nisyros-Tilos volcanic field

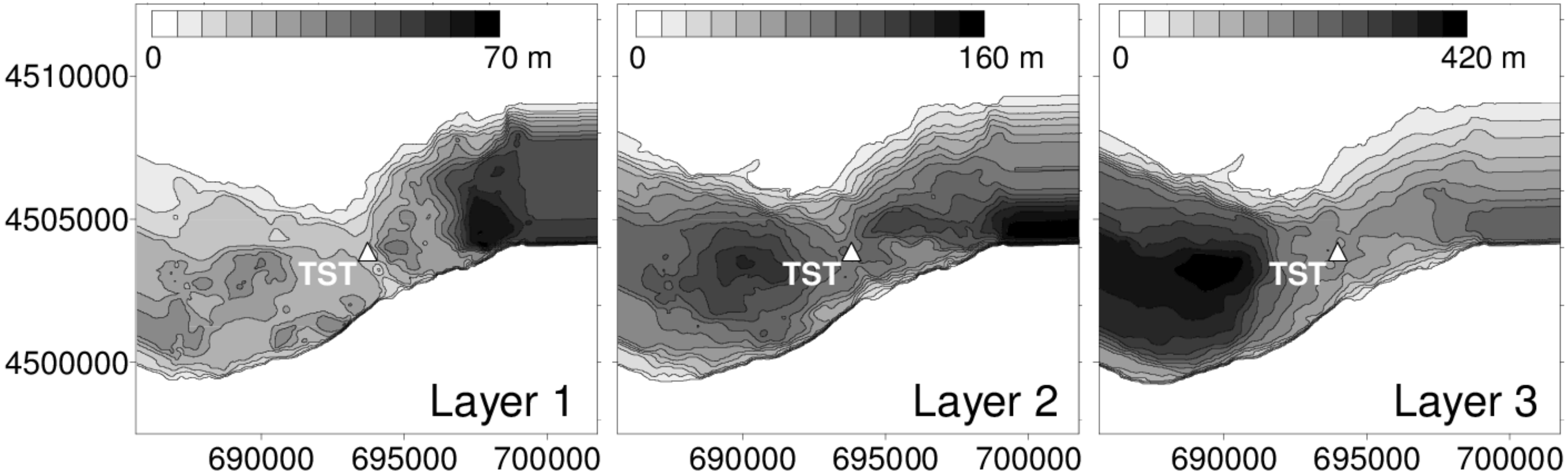
University of Hamburg (UHIG), GeoPro and NOAIG



model of a small (~ 15 km long, ~ 5 km wide)

Mygdonian sedimentary basin near Thessaloniki, Greece

E2VP – Euroseistest Verification and Validation project



Layer	3D Model with homogeneous layers				3D Model with constant-gradient layers				Q_P
	V_S (m/s)	V_P (m/s)	ρ (kg/m^3)	Q_S	V_S (m/s)	V_P (m/s)	ρ (kg/m^3)	Q_S	
1	200	1500	2100	20	200-250	1500-1600	2100	20-25	∞
2	350	1800	2200	35	250-500	1600-2200	2100-2130	25-50	∞
3	650	2500	2200	65	500-900	2200-2800	2130-2250	50-90	∞
Bedrock	2600	4500	2600	260	2600	4500	2600	260	∞

model features to be accounted for

- rheology
  - solid continuum
    - elastic
    - viscoelastic
    - elastoplastic
    - elasto viscoplastic
  - fluid
    - non-viscous
    - viscous
  - two-phase continuum
    - poroelastic
    - poroviscoelastic
- free surface
  - Earth‘s surface curvature
  - local-scale topography
  - planar

model features to be accounted for

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- free surface
  - Earth's surface curvature
  - local-scale topography
  - planar
- material heterogeneity
  - material interface
    - 0th-order
    - 1st-order
  - smooth heterogeneity (gradient)
- isotropy/anisotropy
- physical (computational) domain
  - Earth
    - natural free-surface boundary
  - part of the Earth:
    - artificial boundary
    - natural free-surface boundary

we will restrict the presentation now

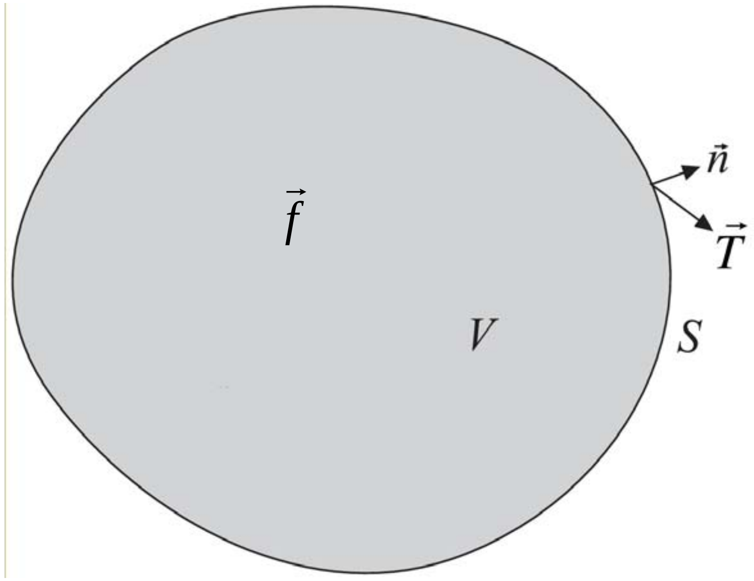
to the problem of

seismic wave propagation

in viscoelastic continuum

governing equations
for elastic and viscoelastic continuum

governing equations for elastic and viscoelastic continuum



material volume V of a smooth continuum
bounded by surface S

body force $\vec{f}$ acts in volume V
external traction $\vec{T}$ acts at surface S

strong form

$$\rho \frac{\partial^2 u_i}{\partial t^2} - \frac{\partial \sigma_{ij}}{\partial x_j} - f_i = 0 \qquad \text{at any point in } V$$

$$T_i = \sigma_{ij} n_j \qquad \text{at any point of } S$$

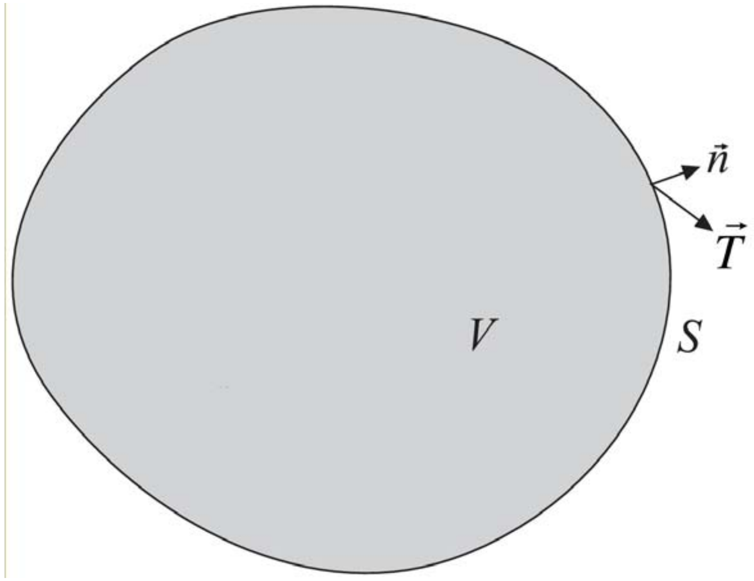
requires continuity of displacement and its first spatial derivatives

weak form

$$\int_V \left(\rho \frac{\partial^2 u_i}{\partial t^2} - f_i \right) w_i \, dV + \int_V \sigma_{ij} \frac{\partial w_i}{\partial x_j} \, dV = \int_S T_i \, w_i \, dS$$

requires continuity of displacement and the weight functions

governing equations for elastic and viscoelastic continuum



material volume V of a smooth continuum
bounded by surface S

body force $\vec{f}$ acts in volume V
external traction $\vec{T}$ acts at surface S

integral strong form

$$\int_V \left(\rho \frac{\partial^2 u_i}{\partial t^2} - \frac{\partial \sigma_{ij}}{\partial x_j} - f_i \right) w_i \, dV = \int_S \left(T_i - \sigma_{ij} n_j \right) w_i \, dS$$

continuity of the first spatial derivative of displacement

governing equations for other media

surface waves at periods $>$ 150 s
are affected by the Earth's rotation

Rayleigh waves
are affected by self-gravitation
(perturbations in the gravitational field
induced by wave propagation)

constitutive relations

for elastic and viscoelastic continuum

constitutive law for elastic and viscoelastic continuum

stress-strain relation in an anisotropic elastic continuum

- Cauchy's generalization of the original Hooke's law

$$\sigma_{ij} = c_{ijkl}\,\varepsilon_{kl}$$

symmetries of elastic constants

$$c_{ijkl} = c_{jikl} \qquad c_{ijkl} = c_{klji} \qquad c_{ijkl} = c_{jilk}$$

21 independent constants in the most general anisotropic medium

stress-strain relation in an isotropic elastic continuum

$$\sigma_{ij}(t) = \delta_{ij}\,\kappa\;\varepsilon_{kk}(t) + 2\mu\left[\varepsilon_{ij}(t) - \tfrac{1}{3}\varepsilon_{kk}(t)\delta_{ij}\right]$$

$$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

stress-strain relation in an isotropic viscoelastic continuum

$$\sigma_{ij}(t) = \delta_{ij}\int_{-\infty}^{t}\kappa(t-\tau)\;\varepsilon_{kk}(\tau)\,d\tau + 2\int_{-\infty}^{t}\mu(t-\tau)\left[\varepsilon_{ij}(\tau) - \frac{1}{3}\varepsilon_{kk}(\tau)\delta_{ij}\right]d\tau$$

strong-form formulations coupling gov. eq. and const. law

displacement-stress

$$\rho \frac{\partial^2 u_i}{\partial t^2} = \frac{\partial \sigma_{ij}}{\partial x_j} + f_i$$

$$\sigma_{ij} = \kappa \varepsilon_{kk} \delta_{ij} + 2\mu \left(\varepsilon_{ij} - \tfrac{1}{3} \varepsilon_{kk} \delta_{ij} \right)$$

displacement-velocity-stress

$$\rho \frac{\partial v_i}{\partial t} = \frac{\partial \sigma_{ij}}{\partial x_j} + f_i \quad , \quad v_i = \frac{\partial u_i}{\partial t}$$

$$\sigma_{ij} = \kappa \varepsilon_{kk} \delta_{ij} + 2\mu \left(\varepsilon_{ij} - \tfrac{1}{3} \varepsilon_{kk} \delta_{ij} \right)$$

velocity-stress

$$\rho \frac{\partial v_i}{\partial t} = \frac{\partial \sigma_{ij}}{\partial x_j} + f_i$$

$$\frac{\partial \sigma_{ij}}{\partial t} = \kappa \frac{\partial \varepsilon_{kk}}{\partial t} \delta_{ij} + 2\mu \left(\frac{\partial \varepsilon_{ij}}{\partial t} - \frac{1}{3} \frac{\partial \varepsilon_{kk}}{\partial t} \delta_{ij} \right)$$

$$\frac{\partial \varepsilon_{ij}}{\partial t} = \frac{1}{2} \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right)$$

boundary and initial conditions

boundary conditions for elastic/viscoelastic continuum

free surface: zero traction

in most applications it is sufficient
to replace air above the Earth's surface by vacuum

consequently, the real Earth's surface
can be considered the traction-free surface

$\vec{T}(\vec{n}) = 0$ that is $\sigma_{ij} n_j = 0$ at a general surface S

$\sigma_{iz} = 0$ at a planar surface perpendicular to z-axis

welded interface: continuity of displacement and traction

$$u_i\big|_{\Sigma^+} = u_i\big|_{\Sigma^-}$$

$$\sigma_{ij} n_j\big|_{\Sigma^+} = \sigma_{ij} n_j\big|_{\Sigma^-}$$

initial conditions

it is usually assumed that the medium at an initial time is at rest

displacement, displacement-stress

$$u_i\left(t=0, x_j\right) = 0 \qquad \frac{\partial^2 u_i}{\partial t^2}\left(t=0, x_j\right) = 0$$

displacement-velocity-stress

$$u_i\left(t=0, x_j\right) = 0 \qquad v_i\left(t=0, x_j\right) = 0$$

velocity-stress

$$v_i\left(t=0, x_j\right) = 0 \qquad \sigma_{ij}\left(t=0, x_k\right) = 0$$

in all cases

$$f_i\left(t=0, x_j\right) = 0$$

exact and approximate methods

there are

analytical or semi-analytical solutions

for relatively very simple/canonical elastic models

of the Earth‘s interior

these solutions are

far from the possibility to explain

the range of wave phenomena

in structurally complex

viscoelastic, anisotropic or poroelastic

models of the Earth‘s interior

approximate methods

only approximate methods
are able to account for
the geometrical and rheological complexity
of the sufficiently realistic models

the most important aspects of each method
are
accuracy and computational efficiency
(in terms of computer memory and time)

these two aspects are in most cases contradictory

the reasonable balance
between the accuracy and computational efficiency
(in case of complex realistic structures)
makes the numerical-modelling methods,
and more specifically, so-called domain (in the spatial sense) methods
dominant among all approximate methods

approximate methods

a variety of the domain numerical methods
has been developed during the last few decades

the best known are
the (time-domain) finite-difference, finite-element,
Fourier pseudo-spectral, spectral-element
and discontinuous Galerkin methods

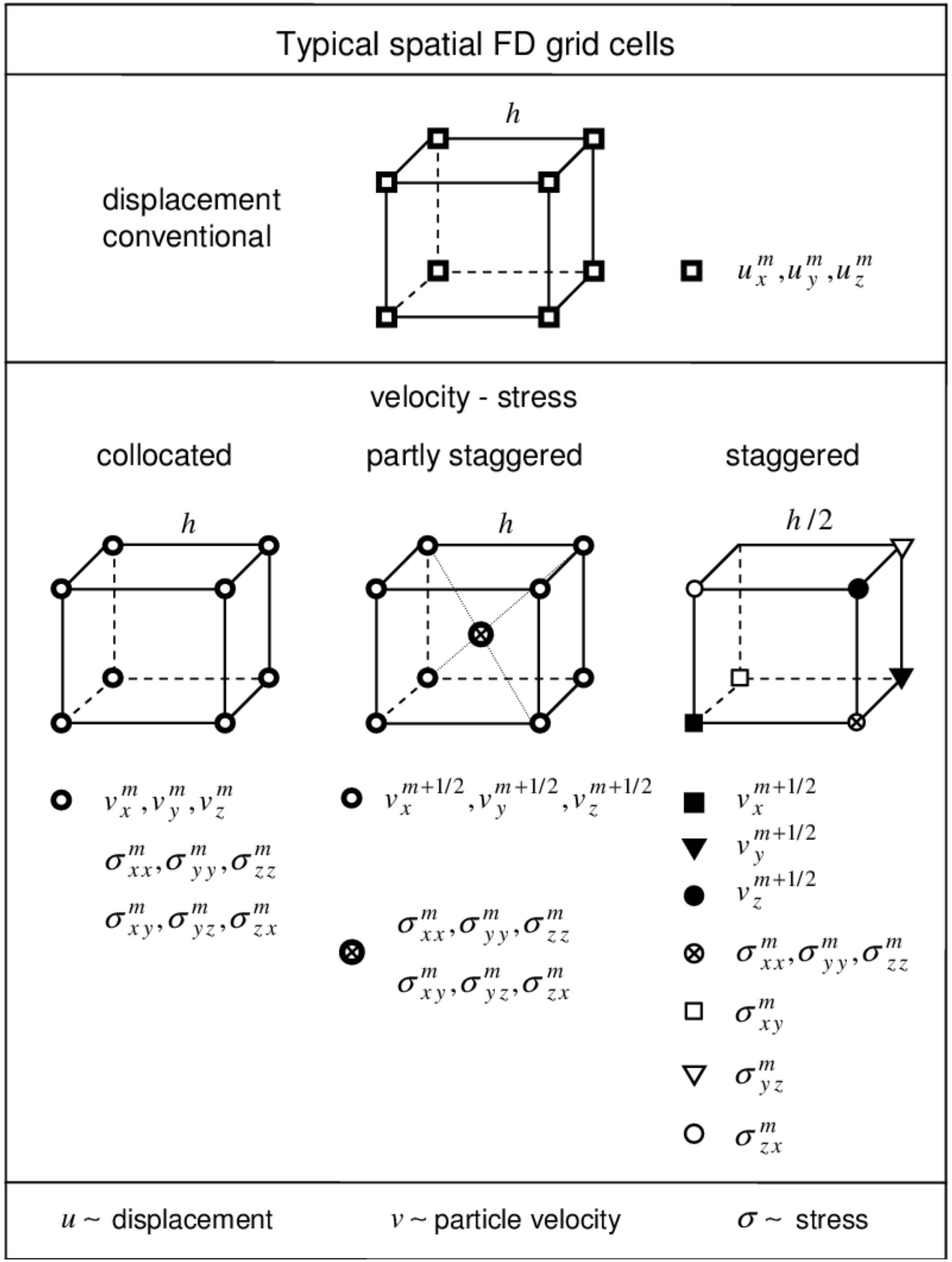
both the theoretical analyses and numerical experience
show that
none of these methods
can be chosen as the universally best method
(in term of accuracy and computational efficiency)
for all important medium-wavefield configurations

each method has its advantages and disadvantages
that often depend on the particular application

FDM - Finite-Difference Method

- construction of a discrete FD model of the problem
  - coverage of the computational domain by a space-time grid
    - uniform, non-uniform, discontinuous grids
    - structured, unstructured grids
    - space-time location of field variables
  - FD approximations of derivatives, functions,
    initial and/or boundary condition at the grid points
    - spatial derivative
      - number of spatial grid positions
      - number of time levels
      - centred/backward/forward/combination
      - order of approximation
      - uniformity/non-uniformity of approx. in diff. spatial directions
    - temporal derivative
      - number of time levels
      - number of spatial positions
      - centred/forward
      - replacement of higher derivatives by spatial derivatives
  - discrete (grid) representation of material properties

    crucial for accuracy with respect to material heterogeneity
  - construction of a system of algebraic equations;
    we may call them FD equations or FD scheme


Typical spatial FD grid cells
displacement conventional
h
u_x^m, u_y^m, u_z^m
velocity - stress
collocated
partly staggered
staggered
h
h
h/2
v_x^m, v_y^m, v_z^m
$\sigma_{xx}^m, \sigma_{yy}^m, \sigma_{zz}^m$
$\sigma_{xy}^m, \sigma_{yz}^m, \sigma_{zx}^m$
$v_x^{m+1/2}, v_y^{m+1/2}, v_z^{m+1/2}$
$\sigma_{xx}^m, \sigma_{yy}^m, \sigma_{zz}^m$
$\sigma_{xy}^m, \sigma_{yz}^m, \sigma_{zx}^m$
$v_x^{m+1/2}$
$v_y^{m+1/2}$
$v_z^{m+1/2}$
$\sigma_{xx}^m, \sigma_{yy}^m, \sigma_{zz}^m$
σ_{xy}^m
σ_{yz}^m
σ_{zx}^m
u ~ displacement
v ~ particle velocity
σ ~ stress

- analysis of the FD model
  - consistency and order of the approximation
  - stability and grid dispersion
  - convergence
  - local error

- numerical computations

analysis of the FD model and numerical computations
may lead to redefinition of the grid and FD approximations
if the numerical behaviour of the developed FD scheme
is not satisfactory

FEM (Finite-Element Method)

and

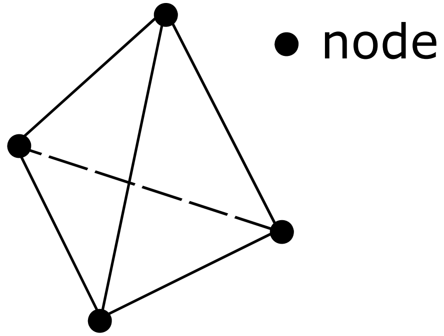
SEM (Spectral-Element Method)

displacement formulation of equation of motion - D-EqM

$$\rho \ddot{u}_i = \sigma_{ij,j} \qquad \sigma_{ij} = \lambda \delta_{ij} u_{k,k} + \mu (u_{i,j} + u_{j,i})$$

choose an element with n nodes

e.g. tetrahedron with 8 nodes (FEM)
hexahedron with 64 nodes (SEM)



choose a shape function and approximation to displacement in the element

$$u_i\left(x_j\right) = s^k\left(x_j\right) U_i^k \quad ; \quad k = 1,\ldots,n$$

U_i^k - unique displacements at nodes

we have to assure continuity of displacement u_i at a contact of elements multiply D-EqM by the shape functions

$$\rho \ddot{u}_i s^k = \sigma_{ij},_j s^k \quad ; \quad k = 1, \ldots, n$$

integrate over an element

$$\int_{\Omega^e} \rho \ddot{u}_i s^k dV = \int_{\Omega^e} \sigma_{ij},_j s^k dV$$

integrate the r.h.s. by parts

$$\int_{\Omega^e} \rho \ddot{u}_i s^k dV = -\int_{\Omega^e} \sigma_{ij} s,_j^k dV + \int_{\partial \Omega^e} T_i s^k dS$$

$$\mathbf{M}^{\mathrm{e}} \ddot{\mathbf{u}}^{\mathrm{e}} = -\mathbf{K}^{\mathrm{e}} \mathbf{u}^{\mathrm{e}} + \text{surface-traction boundary term}$$

local mass matrix

local vector of nodal accelerations

local stiffness matrix

local vector of nodal displacements

$$\mathbf{M}^e \ddot{\mathbf{u}}^e = -\mathbf{K}^e \mathbf{u}^e + \text{surface-traction boundary term}$$

assemble all elements covering volume Ω closed by surface $\partial\Omega$

$$\partial\Omega = \partial\Omega_{FS} \cup \partial\Omega_{\text{Dirichlet}}$$

$$\mathbf{M}\,\ddot{\mathbf{u}} = -\mathbf{K}\,\mathbf{u} + 0$$

- $\mathbf{M}$: global mass matrix
- $\ddot{\mathbf{u}}$: global vector of nodal accelerations
- $\mathbf{K}$: global stiffness matrix
- $\mathbf{u}$: global vector of nodal displacements

the theoretical boundary term vanishes
- at a contact of two elements - due to traction continuity
- at the free surface - due to zero traction

in fact, however, the final discretization does not give exactly
- the traction continuity at a contact of two elements
- zero traction at the free surface

and thus the zero boundary term in the global equation

they are just (possibly low-order) approximated

general notes
on implementation of FEM/SEM

shape of an element, number of nodes
and their positions in an element
are related to the shape functions

integrals in previous formulas
are usually evaluated numerically
using different quadratures

though different combinations of
shape functions and quadrature are possible,
each combination affects properties
of the resulting scheme/method

FEM	SEM
shape functions and quadrature are independent	shape functions and quadrature are closely related; the approach minimizes numerical dispersion and dissipation
shape functions	
(usually) Lagrange polynomials	Legendre polynomials
integration / numerical quadrature	
usually Gauss quadrature for its efficiency; in principle any quadrature with required/desired accuracy	Gauss-Lobatto-Legendre quadrature with integration points coinciding with node positions; leads to a diagonal mass matrix
shape of an element	
wide range of shapes, e.g., tetrahedra, hexahedra, pyramids…	usually hexahedral elements in 3D, quadrilateral elements in 2D

ADER-DGM

(Arbitrarily high-order DERivative

Discontinuous Galerkin Method)

velocity-stress formulation of equation of motion - VS-EqM

$$\dot{\sigma}_{ij} - \lambda v_{k,k} \delta_{ij} - \mu (v_{i,j} - v_{j,i}) = 0$$

$$\rho \dot{v}_i - \sigma_{ij,j} = 0$$

define a vector of unknown variables

$$Q = \left(\sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \sigma_{xy}, \sigma_{yz}, \sigma_{zx}, v_x, v_y, v_z\right)^T$$

VS-EqM in the matrix form

$$\dot{Q}_p + A_{pq} Q_{q,x} + B_{pq} Q_{q,y} + C_{pq} Q_{q,z} = 0$$

A, B, C space-dependent matrices include material properties

tetrahedral element (e.g.)

$$(Q_h)_p = \hat{Q}_{pk}(t)\, \Phi_k(x_j)$$

Φ_k — polynomial basis functions of an optional degree multiply VS-EqM by a test function and integrate over an element volume

$$\int_{\Omega^e} \dot{Q}_p \Phi_k \, dV + \int_{\Omega^e} \left(A_{pq} Q_{q,x} + B_{pq} Q_{q,y} + C_{pq} Q_{q,z} \right) \Phi_k \, dV = 0$$

integrate the 2nd integral by parts

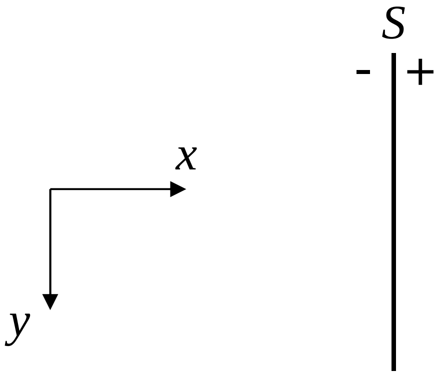
$$\int_{\Omega^e} \dot{Q}_p \Phi_k \, dV - \int_{\Omega^e} \left(\Phi_{k,x} A_{pq} + \Phi_{k,y} B_{pq} + \Phi_{k,z} C_{pq} \right) Q_q \, dV + \int_{\partial\Omega^e} \Phi_k F_p \, dS = 0$$

numerical flux introduced
because Q_h may be discontinuous
at an element boundary

Riemann problem – an evolution physically continuous problem
with initial discontinuous approximation of unknowns
across an interface

to find a flux such that
continuity of particle velocity and traction
at an element boundary is assured

2D illustration of solution of the Riemann problem



S – interface of two triangular elements perpendicular to the x-axis

the Riemann problem is exactly solved by the Godunov state

$$Q_P^G = Q_P\left(S^-\right) = Q_P\left(S^+\right)$$

for example :

$$Q_3^G = \sigma_{xy}^G = \frac{1}{2}\left[\left(\sigma_{xy}^- - \sigma_{xy}^+\right) + \frac{\mu}{c_S}\left(v_y^- - v_y^+\right) \right]$$

$$Q_5^G = v_y^G = \frac{1}{2}\left[\frac{c_S}{\mu}\left(\sigma_{xy}^- - \sigma_{xy}^+\right) + \left(v_y^- - v_y^+\right) \right]$$

	FDM	SEM	ADER-DGM
brief characterization	the most intuitive and thus relatively easy; the name represents a large variety of formulations and schemes of very different properties (accuracy and efficiency)	combines accuracy of global pseudospectral method with flexibility of FEM; usually uses hexahedral elements	relatively universal with respect to model geometrical and rheological complexity, optional level of accuracy (equal in space and time), p and h adaptivity; uses tetrahedral elements
aspect			
computational domain			
whole Earth	not yet well applicable (problems with gridding and free surface)	the most successful so far compared to other methods	presently not applicable (too large computational demands)
region (tens to hundreds of km)	relatively applicable	very suitable	relatively applicable
local structure (hundreds of m to km)	intensively applied, efficient	well applicable with comp. demands strongly depending on material heterogeneity and meshing	
seismic exploration models (hundreds of m to km)			
free surface	not trivial	implicit and natural	
smooth heterogeneity	feasible – depends on discrete representation of material properties	possible – strongly depends on polynomial degree	
material interface	efficient with very good level of accuracy if material properties are properly represented in a grid; does not need conforming grids	if element boundaries do not follow an interface, there is a problem with accuracy; the following of an interface (honouring geometry) can significantly increase computational demands and is not easy with hexahedral elements	if element boundaries do not follow an interface, there is a problem with accuracy; the following of an interface (honouring geometry) can significantly increase computational demands
viscoelasticity	easy, increases mainly demands on computer memory		
poroelasticity	applicable		applicable, very good level of accuracy
anisotropy	uneasy for schemes other than on a collocated grid	easy	

Lessons learned from ESG2006 and E2VP

Methodological – general

- There is no single numerical-modeling method
  that can be considered the best – in terms of accuracy and computational efficiency – for all structure-wavefield configurations

- Apparently/intuitively “small” or “insignificant” differences
  in the discrete representation of spatial variation in material parameters
  can cause considerable inaccuracies and consequently discrepancies

- Sufficiently accurate and computationally efficient methods
  for implementing
  - continuous and discontinuous material heterogeneity
  (consistent with the interface boundary condition),
  - realistic attenuation (not simpler than that corresponding to the GZB/GMB-EK rheology),
  - nonreflecting boundary (not less efficient than PML)
  - free-surface condition
  prove to be the key elements
  of a reasonably accurate numerical simulation

Lessons learned from ESG2006 and E2VP

Methodological – finite-difference method

The commonly used name of "finite-difference method"
in the numerical modeling of earthquake ground motion
may represent one of a large variety of FD schemes and codes

Surprisingly,
not all FD schemes
used for simulations and publications
are at the state-of-the-art level

Lessons learned from ESG2006 and E2VP

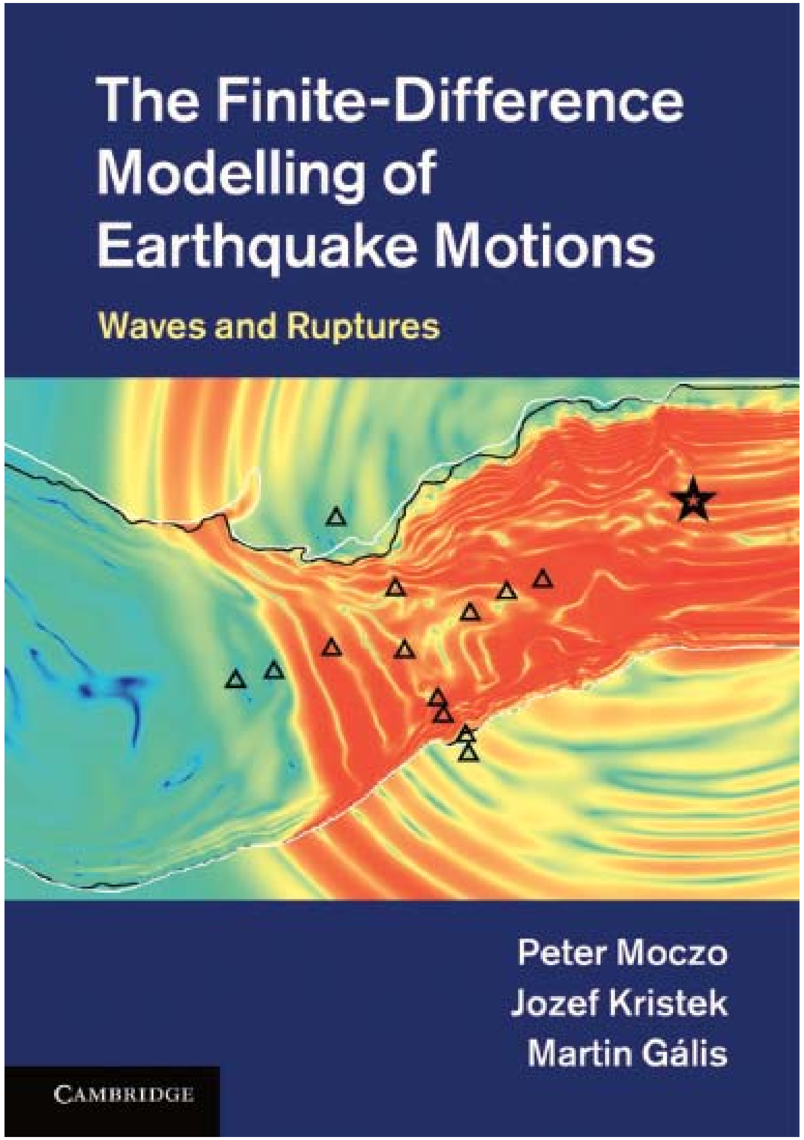
Practical

The numerical-simulation methods
and the corresponding computer codes
are not yet in a “press-button” mode;
the codes should never be applied as black-box tools,
that is,
without sufficient methodological knowledge
of the method and the code

At least two different but comparably accurate,
verified and state-of-the-art methods
should be applied
in order to obtain reliable numerical prediction
of earthquake ground motion at a site of interest

Material interfaces
should not be artificially introduced
in the computational model;
their presence can have strong impact
on the locally induced surface waves

It is necessary to perform numerical simulations
for at least two different discretizations



www.cambridge.org/moczo

FDSim

The Fortran95 Codes
for Numerical Simulation
of Seismic Wave Propagation
in Heterogeneous Viscoelastic Media

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Support for FDSim3D Please, post here questions/comments related to using the FDSim3D package. **Subforums:** Download, Compile, Run simulations, Other	0	0	No posts
SISMOWINE In addition to the resources, you may find it useful to visit SISMOWINE - an open interactive seismological web interface used for numerical-modelling benchmarking.			

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STATISTICS

Total posts **7** • Total topics **7** • Total members **35** • Our newest member **kadmiel**

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