2024 Workshop
Numerical Modeling of Earthquake Motions: Waves and Ruptures

Finite-Difference Numerical Simulation of Seismic Waves Propagation in Models with Complex Boundary Geometries

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Finite-difference method (FDM)

Governing equation

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

$$\frac{\partial \sigma_{ij}}{\partial t} = \lambda \delta_{ij} \frac{\partial v_k}{\partial x_k} + \mu \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right)$$

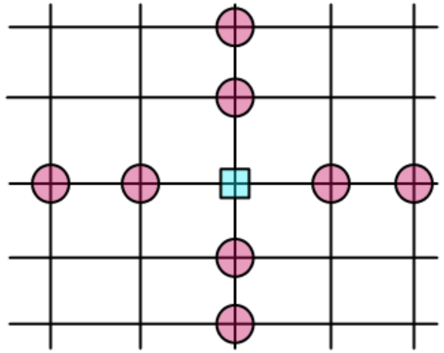
FD discretization

$$\frac{\partial v_i}{\partial t} \sim \frac{v_i^{n+1} - v_i^n}{\Delta t}$$

$$\frac{\partial \sigma_{xy}}{\partial x} \sim \frac{\sigma_{xy}\left(+\frac{\Delta x}{2}\right) - \sigma_{xy}\left(-\frac{\Delta x}{2}\right)}{\Delta x}$$

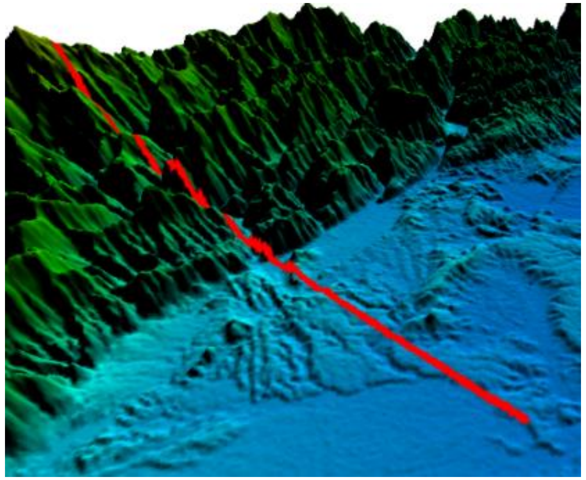
$$\frac{\partial \sigma_{xy}}{\partial y} \sim \frac{\sigma_{xy}\left(+\frac{\Delta y}{2}\right) - \sigma_{xy}\left(-\frac{\Delta y}{2}\right)}{\Delta y}$$

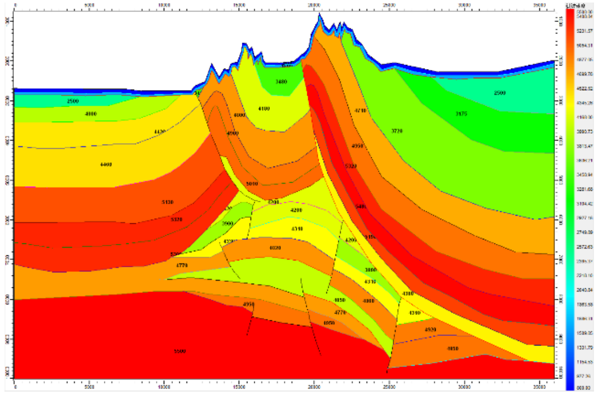
- theory is straightforward
- gridded complex velocity structures
- computational efficiency
- easy to be used



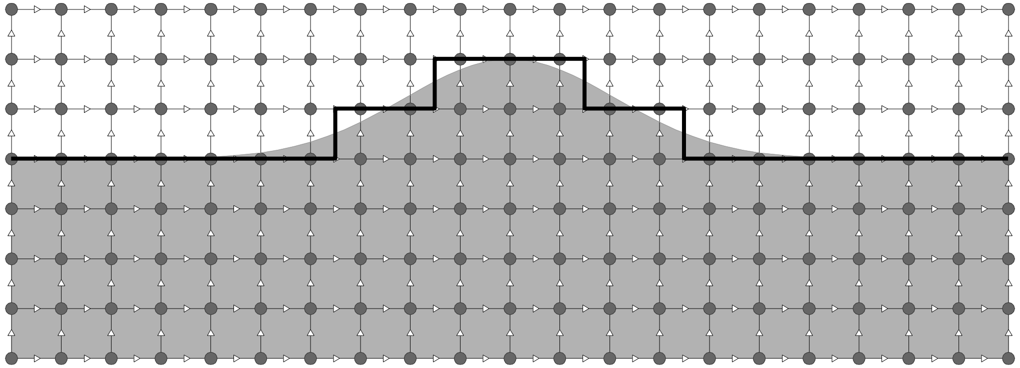
Limitation of early FDM: can’t deal with topography

Surface topography





Using Cartesian grid to approximate topography: staircase shape



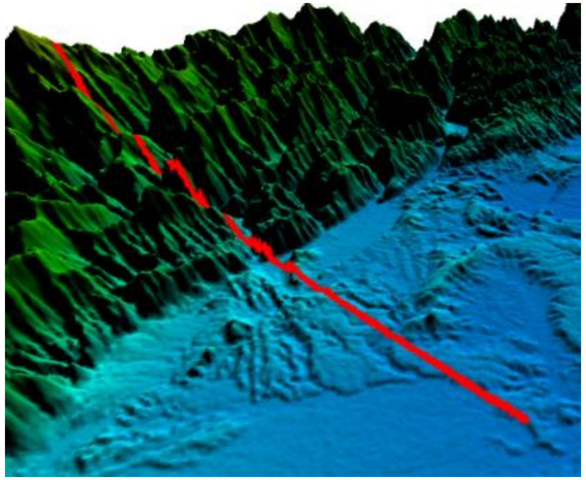
- Zahradník and Urban, 1984
- Frankel and Leith, 1992,
- Robertsson, 1996
- Opršal and Zahradník, 1999
- Hayashi et al., 2001
- Zeng et al., 2012

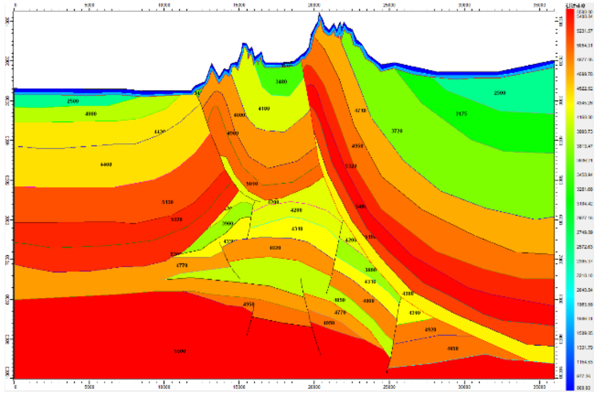
Very dense grid is required (~60 PPW for surface wave)

(Bohlen and Saenger, 2006)

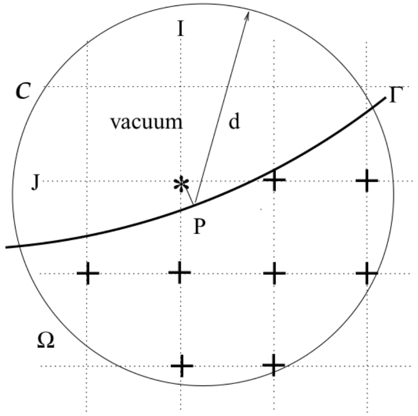
Limitation of early FDM: can't deal with topography

Surface topography

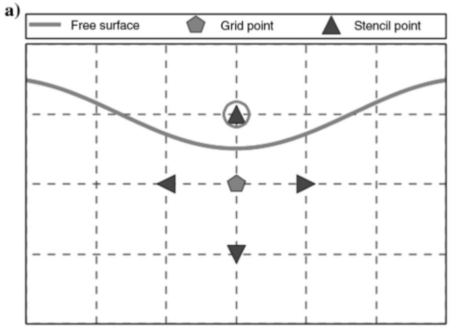




Using Cartesian grid with immersed boundary treatment



Lombard et al., 2008



Gao et al., 2015

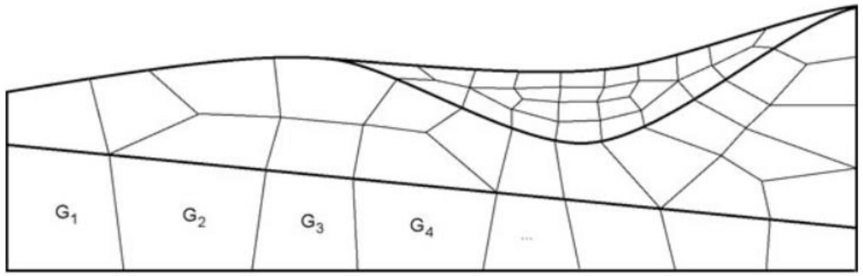
set values above free surface according to analytical condition
hard to code for 3D and stability problem

Limitation of Cartesian grids, but not FDM

FDM not limited to Cartesian grid, but structural grids

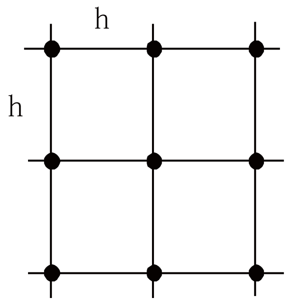
unstructured grid

structural grid

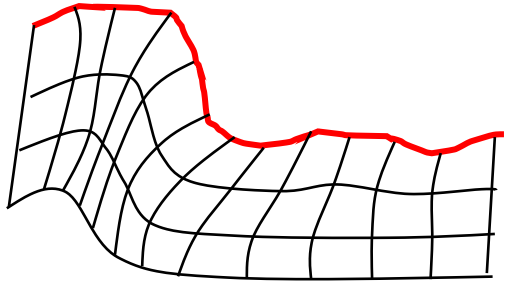


(Fichtner, 2011)

Cartesian grid



curvilinear grid
boundary-conforming grid



- handle boundary and internal complex interfaces
- element conforming to the interfaces
- professional CAD software
- professional grid generation software

- very easy to generate (x0, dx, nx)
- dense grid to represent surface topography

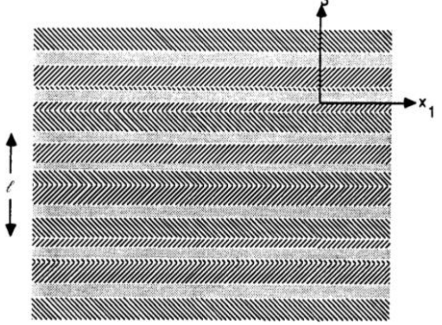
- can represent surface topography well
- very easy to professional grid generation software

FDM only requires the grid to conform to the free surface but not the internal interfaces

effective medium parameterization of the internal interfaces

- grid averaging (Graves, 1996)
- volume averaging (Moczo et al., 2002)
- Orthorhombic medium representation (Moczo et al., 2002, 2014, 2019; Kristek et al., 2017)
- TTI equivalent medium parameterization (Jiang and Zhang, 2021; Koene et al., 2022)

thin isotropic layers



wavelength much larger than thickness

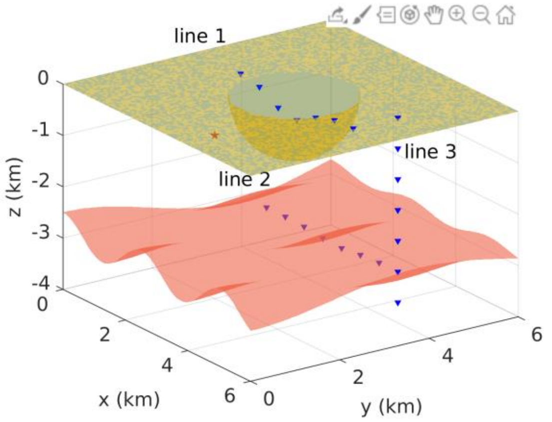
a single layer can produce equivalent stress-strain

VTI anisotropic medium

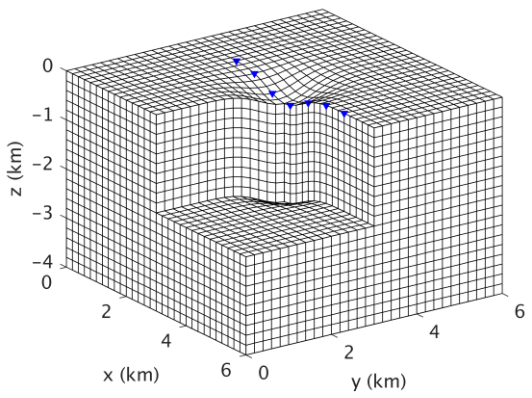
long-wave equivalent theory (Backus,1962)

PPW~5 using TTI effective media

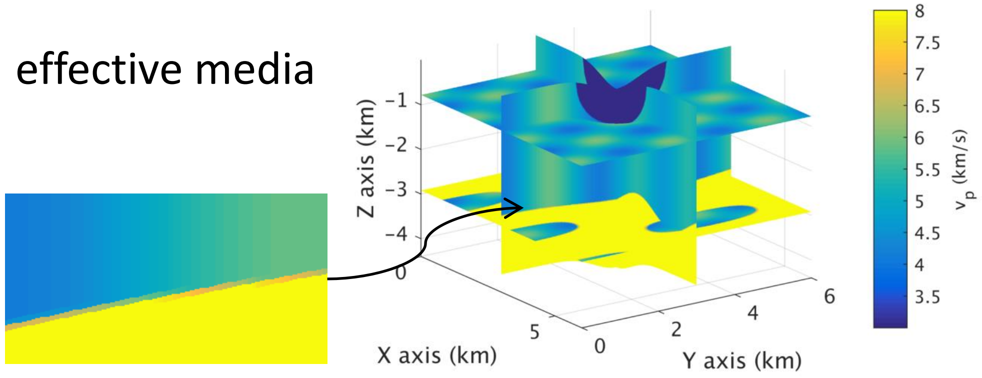
input model

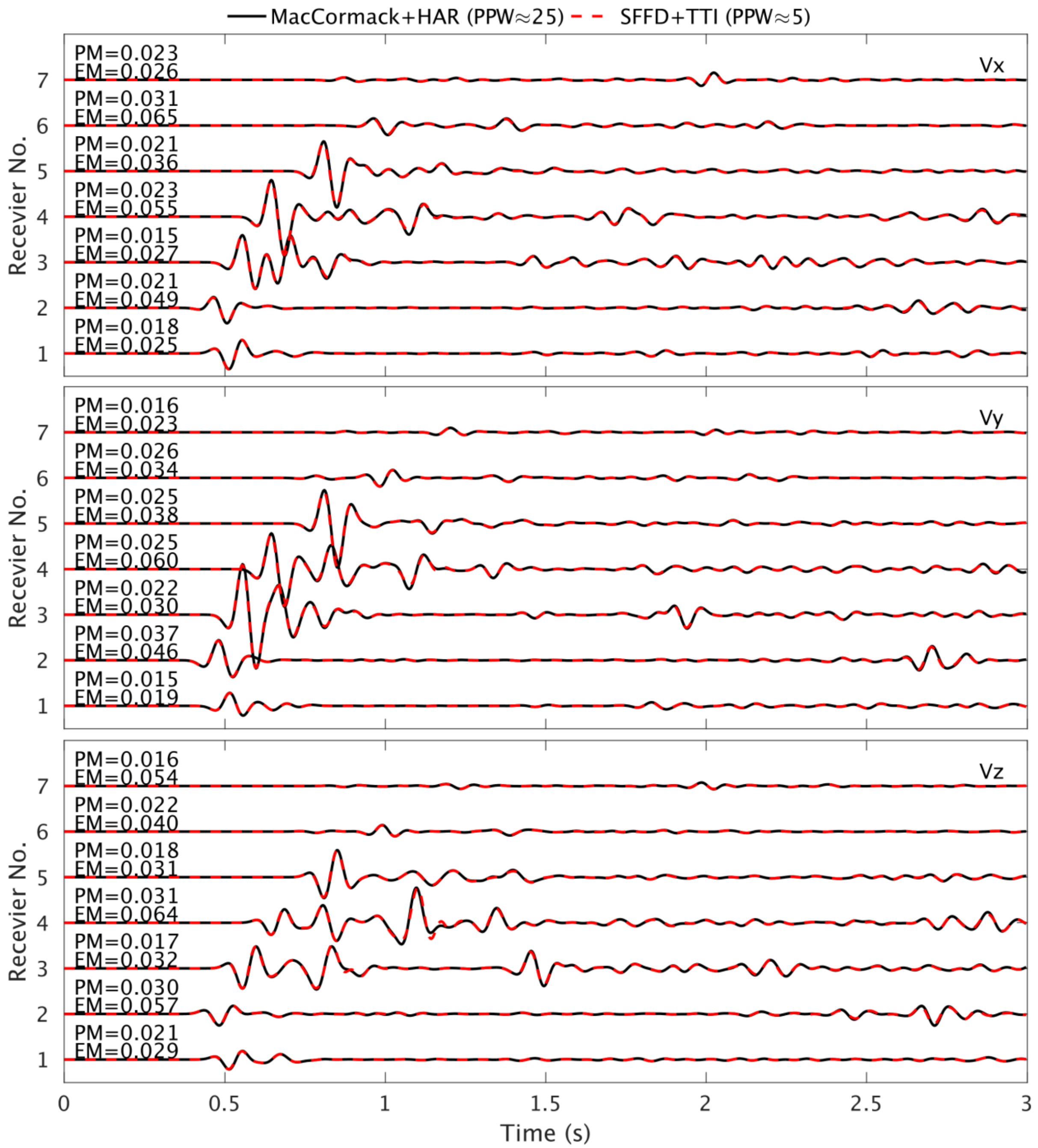


FD grid

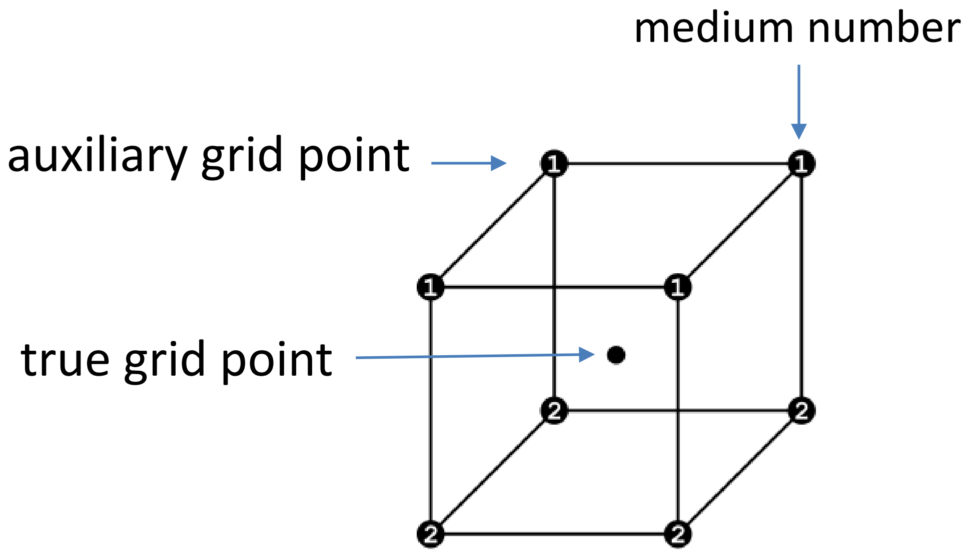


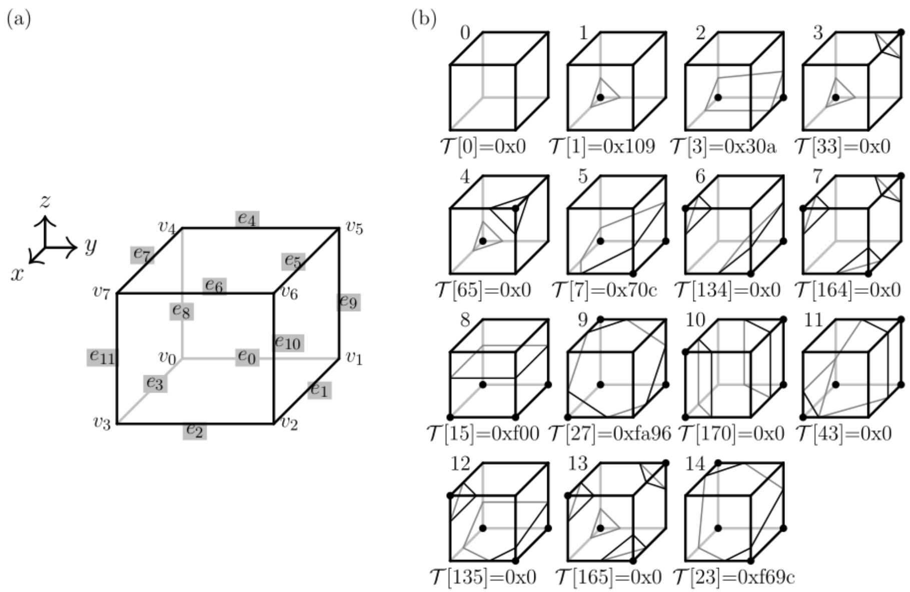
effective media





Efficient method to evaluate effective medium in 2D and 3D





use an auxiliary grid to identify which point should be calculated

use Marching Cube method to calculate volume and normal direction

Jiang, L., and W. Zhang, Efficient implementation of equivalent medium parameterization in finite-difference seismic wave simulation methods, GJI, minor revision

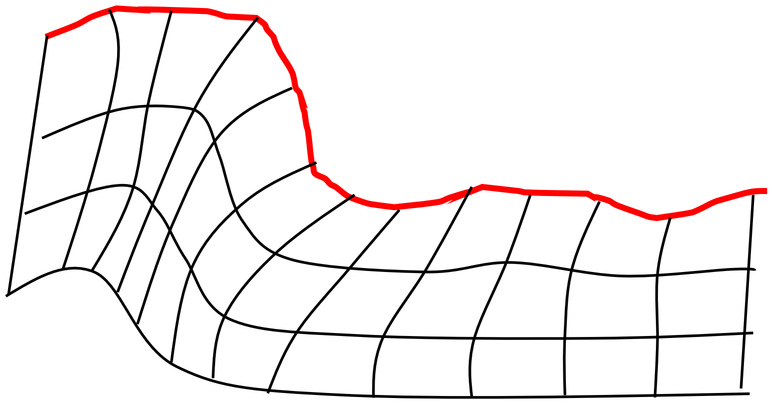
https://github.com/jianglq6/FD3D_ModelPrepare

TOC

Governing equation in curvilinear grid

Momentum equation: $\rho \frac{\partial \mathbf{v}}{\partial t} = \nabla \cdot \boldsymbol{\sigma} + \mathbf{f}$

- curvilinear grid represents a general curvilinear coordinate



physical coordinate (x, z)

computational/
curvilinear coordinate (ξ, ζ)

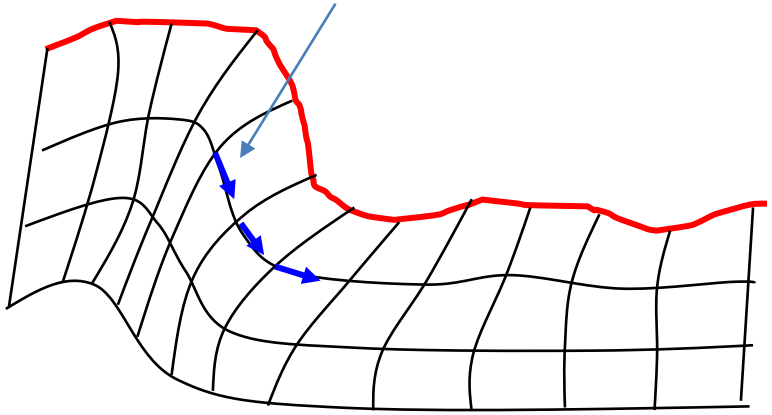
- spatial derivatives are evaluated along the curvilinear grid lines
- Wavefield variables can be defined in two different ways

1. direction of components along the general coordinates
2. direction of components along the global Cartesian coordinate

Governing equation: $$\rho \frac{\partial \mathbf{v}}{\partial t} = \nabla \cdot \boldsymbol{\sigma} + \mathbf{f}$$

1. variables are defined in the general coordinates (Tensorial formulation)

Base vector/direction varies point by point



$$\mathbf{v} = v^i \mathbf{e}_i$$

$$\rho \frac{\partial v^i}{\partial t} = \sigma^{ij}{}_{,j} + \sigma^{ih}\Gamma^j_{hj} + \sigma^{hj}\Gamma^i_{jh} + X^i$$

Christoffel symbols

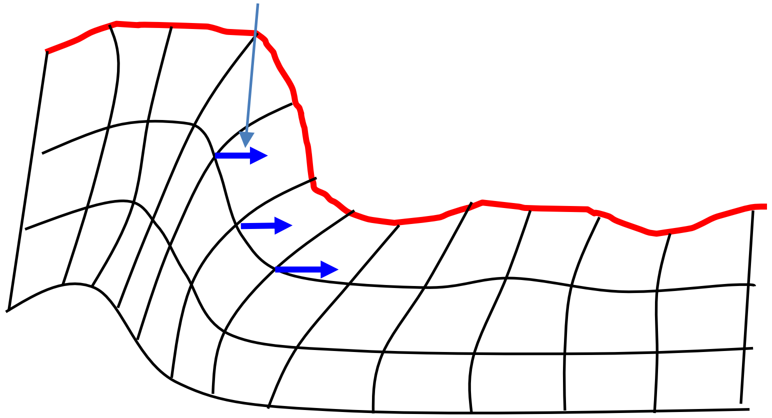
18 components per point!

(Komatitsch et al., 1996; Shragge and Konuk, 2020)

Governing equation: $\rho \frac{\partial \mathbf{v}}{\partial t} = \nabla \cdot \boldsymbol{\sigma} + \mathbf{f}$

2. variables are defined in the global Cartesian coordinates

Base vector/direction is invariant



$$\mathbf{v} = v_i \mathbf{i}_i$$

Cartesian coordinate

$$\rho v_{x,t} = \sigma_{xx,x} + \sigma_{xz,z}$$

$\Downarrow$

Chain-rule $\frac{\partial}{\partial x} = \frac{\partial}{\partial \xi}\frac{\partial \xi}{\partial x} + \frac{\partial}{\partial \zeta}\frac{\partial \zeta}{\partial x}$

$\Downarrow$

curvilinear coordinate

$$\rho v_{x,t} = \xi_{,x}\sigma_{xx,\xi} + \zeta_{,x}\sigma_{xx,\zeta} + \xi_{,z}\sigma_{xz,\xi} + \zeta_{,z}\sigma_{xz,\zeta}$$

Cartesian coordinate | Curvilinear coordinate

$$
\begin{aligned}
\rho v_{x,t} &= \sigma_{xx,x} + \sigma_{xz,z} + f_x, \\
\rho v_{z,t} &= \sigma_{xz,x} + \sigma_{zz,z} + f_z, \\
\sigma_{xx,t} &= (\lambda + 2\mu) v_{x,x} + \lambda v_{z,z}, \\
\sigma_{zz,t} &= \lambda v_{x,x} + (\lambda + 2\mu) v_{z,z}, \\
\sigma_{xz,t} &= \mu (v_{x,z} + v_{z,x}),
\end{aligned}
$$

$\Rightarrow$

$$
\begin{aligned}
\rho v_{x,t} &= \xi_{,x}\sigma_{xx,\xi} + \xi_{,z}\sigma_{xz,\xi} + \zeta_{,x}\sigma_{xx,\zeta} + \zeta_{,z}\sigma_{xz,\zeta}, \\
\rho v_{z,t} &= \xi_{,x}\sigma_{xz,\xi} + \xi_{,z}\sigma_{zz,\xi} + \zeta_{,x}\sigma_{xz,\zeta} + \zeta_{,z}\sigma_{zz,\zeta}, \\
\sigma_{xx,t} &= (\lambda + 2\mu)\xi_{,x} v_{x,\xi} + \lambda \xi_{,z} v_{z,\xi} \\
&\quad + (\lambda + 2\mu)\zeta_{,x} v_{x,\zeta} + \lambda \zeta_{,z} v_{z,\zeta}, \\
\sigma_{zz,t} &= \lambda \xi_{,x} v_{x,\xi} + (\lambda + 2\mu)\xi_{,z} v_{z,\xi} \\
&\quad + \lambda \zeta_{,x} v_{x,\zeta} + (\lambda + 2\mu)\zeta_{,z} v_{z,\zeta}, \\
\sigma_{xz,t} &= \mu \left(\xi_{,z} v_{x,\xi} + \xi_{,x} v_{z,\xi} + \zeta_{,z} v_{x,\zeta} + \zeta_{,x} v_{z,\zeta} \right).
\end{aligned}
$$

$$\mathbf{W}_{,t} = \mathbf{A}\mathbf{W}_{,x} + \mathbf{B}\boldsymbol{W}_{,z} \qquad \mathbf{W}_{,t} = \mathbf{A}\mathbf{W}_{,\xi} + \mathbf{B}\boldsymbol{W}_{,\zeta}$$

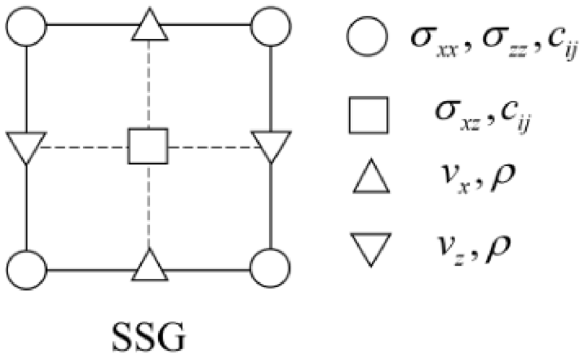
the structure of the equations is similar, with additional differential terms

FD schemes for equations on curvilinear grids

$$\rho v_{x,t} = \xi_{,x}\sigma_{xx,\xi} + \zeta_{,x}\sigma_{xx,\zeta} + \xi_{,z}\sigma_{xz,\xi} + \zeta_{,z}\sigma_{xz,\zeta}$$

staggered-grid schemes: variables are defined at staggered positions

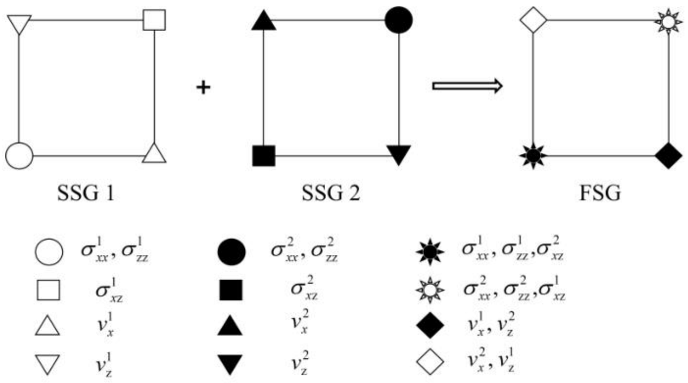
staggered grid



interpolation

Igel et al. (1995)

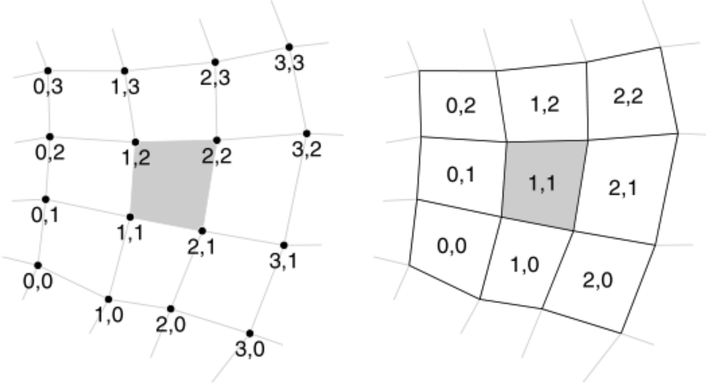
Lebedev grid
full staggered grid



calculate by another staggered grid

Lisitsa and Vishnevskiy (2010)

supporting operator
mimetic scheme



pair of gradient and divergence operators

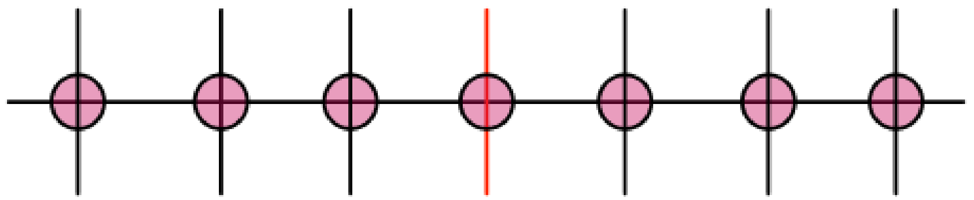
Ely et al. (2006);
Shragge and Tapley (2017)

FD schemes for equations on curvilinear grids

$$\rho v_{x,t} = \xi_{,x}\sigma_{xx,\xi} + \zeta_{,x}\sigma_{xx,\zeta} + \xi_{,z}\sigma_{xz,\xi} + \zeta_{,z}\sigma_{xz,\zeta}$$

collocated-grid schemes: variables are defined at same positions

$$\frac{\partial v_x}{\partial x}\Big|_i \sim \frac{v_x\big|_{i+1} - v_x\big|_{i-1}}{2\Delta x}$$



central difference on collocated grid has a serious odd-even decoupling problem

FD schemes for equations on curvilinear grids

$$\rho v_{x,t} = \xi_{,x}\sigma_{xx,\xi} + \zeta_{,x}\sigma_{xx,\zeta} + \xi_{,z}\sigma_{xz,\xi} + \zeta_{,z}\sigma_{xz,\zeta}$$

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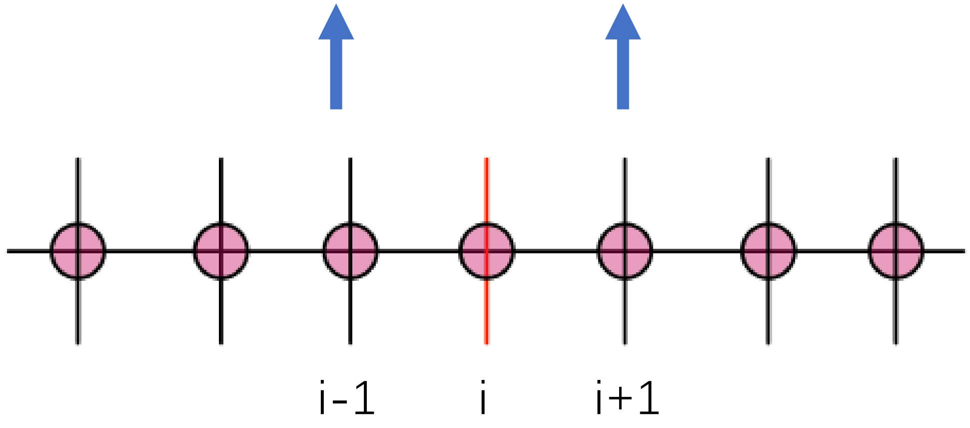

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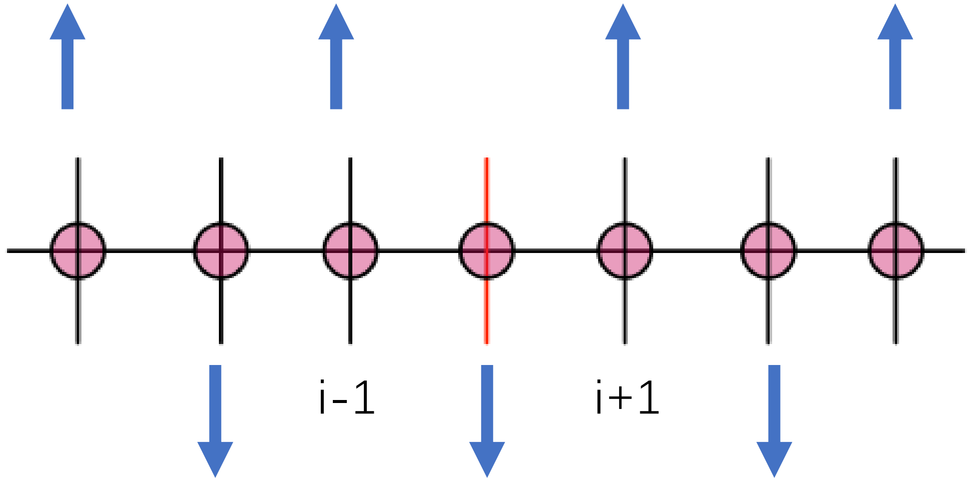

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FD schemes for equations on curvilinear grids

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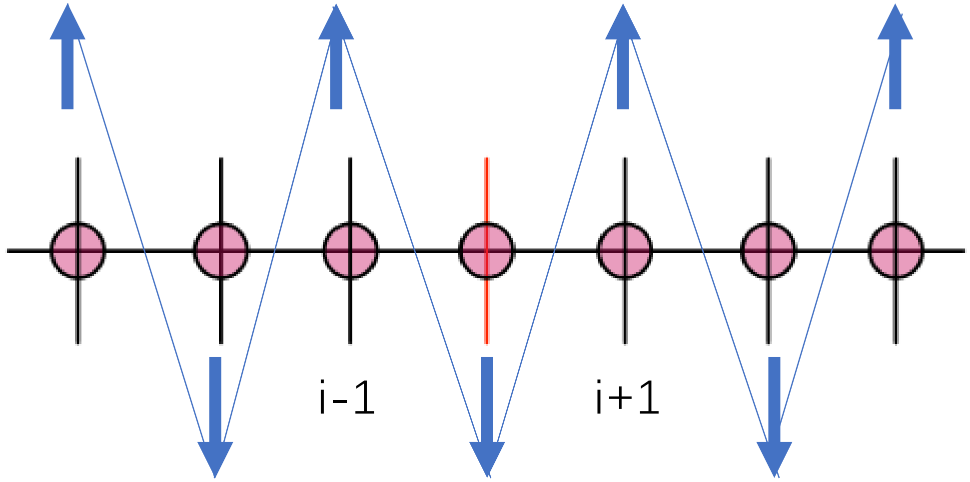


central difference on collocated grid has a serious odd-even decoupling problem

FD schemes for equations on curvilinear grids

3 solutions of odd-even decoupling on collocated-grid FD scheme:

(1) centered difference + explicit filtering

$$\frac{\partial \boldsymbol{U}_i}{\partial \xi} = \frac{1}{\Delta \xi} \sum_{m=1}^{6} a_m \left(\boldsymbol{U}_{i+m} - \boldsymbol{U}_{i-m} \right),$$

$$f(\boldsymbol{U}_i)^d = \boldsymbol{U}_i - \sigma d_0 \boldsymbol{U}_i - \underbrace{\sigma \sum_{m=1}^{6} d_m \left(\boldsymbol{U}_{i+m} + \boldsymbol{U}_{i-m} \right)}_{\text{filter to remove high wavenumber}}$$

(Bogey & Bailly 2006)

(2) centered difference +inherent dissipation

Lax-wendroff scheme

$$\partial_t u + \partial_x f(u) = 0$$

$$\Downarrow$$

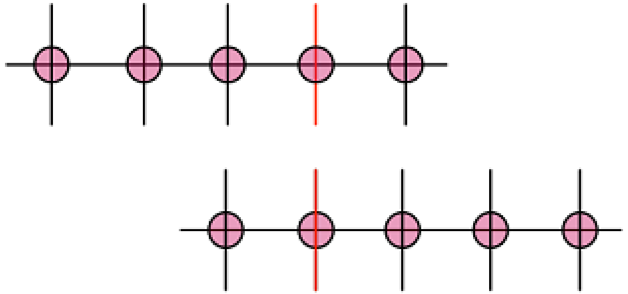
$$u(x_i, t^{n+1}) = u(x_i, t^n) + \\ -\Delta t a \partial_x^{(1)} u(x_i, t^n) + \frac{\Delta t^2}{2} a^2 \partial_x^{(2)} u(x_i, t^n) + O(\Delta t^2)$$

dissipation term

https://encyclopediaofmath.org/wiki/Lax-Wendroff_method

FD schemes for equations on curvilinear grids

3 solutions:



(3) MacCormack-type schemes

$$D_x^F v_{x|i} = \frac{1}{\Delta x}\left(a_3 v_{x|i+3} + a_2 v_{x|i+2} + a_1 v_{x|i+1} + a_0 v_{x|i} + a_{-1} v_{x|i-1}\right)$$

biased forward operator

$$D_x^B v_{x|i} = \frac{1}{\Delta x}\left(-a_{-1} v_{x|i+1} - a_0 v_{x|i} - a_1 v_{x|i-1} - a_2 v_{x|i-2} - a_3 v_{x|i-3}\right)$$

biased backward operator

$$D_x v_{x|i} = \frac{1}{2}\left(D_x^F v_{x|i} + D_x^B v_{x|i}\right) \quad \text{if second order RK used}$$

center difference is recovered

asymmetric stencil has both dispersion and dissipation errors

(Bayliss et al., 1986; Zhang and Chen, 2006; Zhang et al., 2012)

Free surface boundary condition

characteristic boundary condition

decomposition of the wave equation into incoming and outgoing wave modes at subdomain boundaries

$$\mathbf{W}_{,t} = \mathbf{A}\mathbf{W}_{,x} + \mathbf{B}\boldsymbol{W}_{,z}$$

$$\mathbf{B} = \mathbf{S}\boldsymbol{\Lambda}\mathbf{S}$$

$\Rightarrow$

c_s c_p 0

$$R_1 = \sqrt{\rho\mu}\, v_x + \sigma_{xz}$$

$$R_2 = \sqrt{(\lambda + 2\mu)\rho}\, v_z + \sigma_{zz}$$

$$R_3 = (\lambda + 2\mu)\sigma_{xx} - \mu\sigma_{zz}$$

$\Rightarrow$

$$\sigma_{xz}^{(new)} = 0$$

$$\sigma_{zz}^{(new)} = 0$$

$$\sigma_{xx}^{(new)} = \sigma_{xx} - \frac{\lambda}{\lambda + 2\mu}\sigma_{zz}$$

$$v_x^{(new)} = v_x - \frac{\sigma_{zz}}{\sqrt{\mu\rho}}$$

$$v_z^{(new)} = v_z - \frac{\sigma_{zz}}{\sqrt{(\lambda + 2\mu)\rho}}$$

(Gottlieb, 1982; Bayliss et al., 1986; Carcione, 1991)

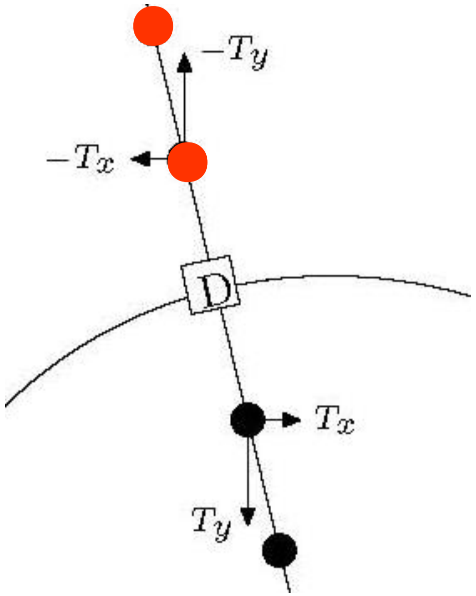
Free surface boundary condition

Traction imaging technique

$$\rho v_{x,t} = \xi_{,x}\sigma_{xx,\xi} + \xi_{,z}\sigma_{xz,\xi} + \zeta_{,x}\sigma_{xx,\zeta} + \zeta_{,z}\sigma_{xz,\zeta},$$

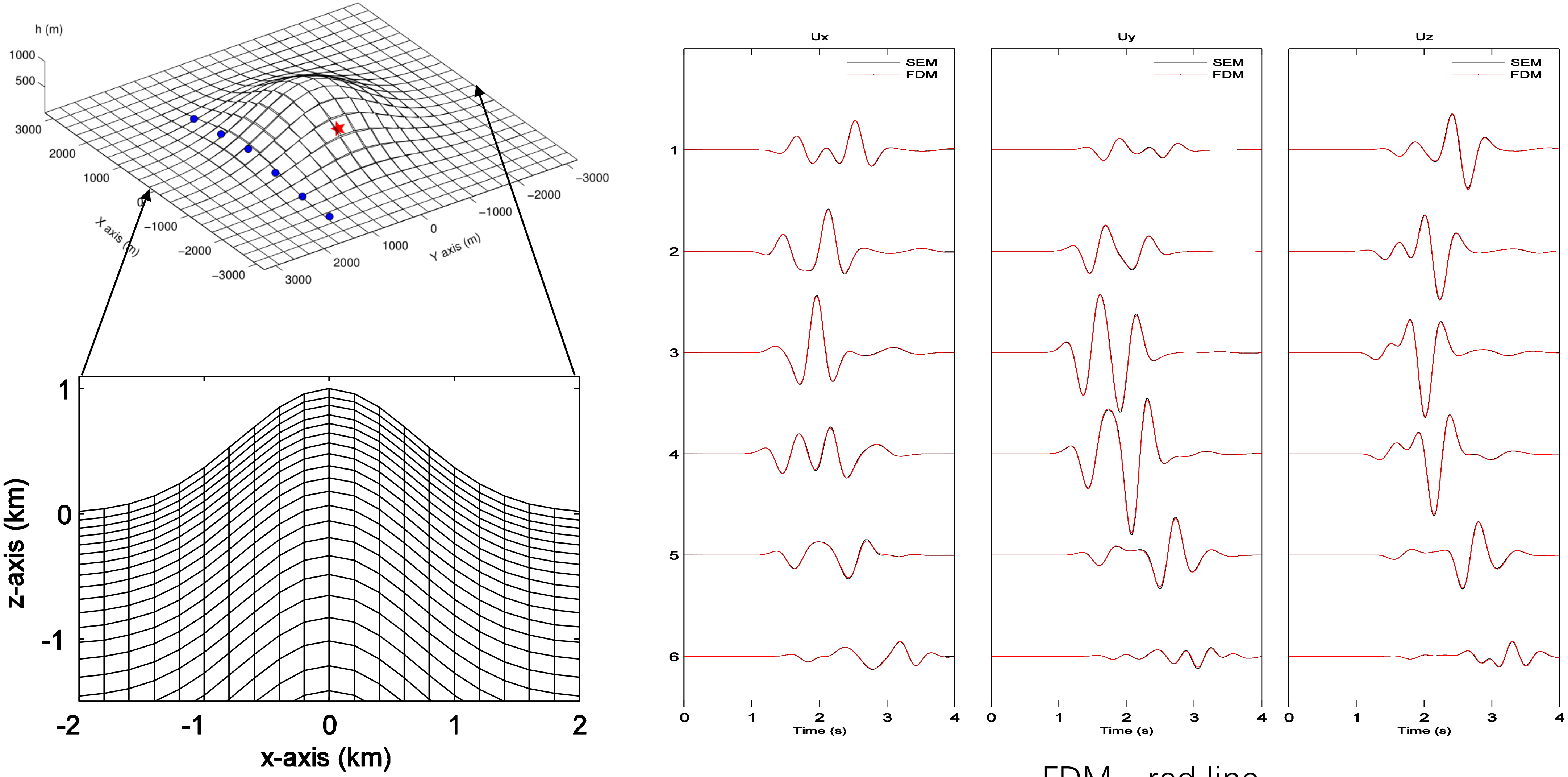
⇓ rewrite using conservative form of ∇

$$\rho\frac{\partial v_x}{\partial t} = \frac{1}{J}\left\{\frac{\partial}{\partial \xi}\left[J\left(\frac{\partial \xi}{\partial x}\sigma_{xx} + \frac{\partial \xi}{\partial z}\sigma_{xz}\right)\right] + \frac{\partial}{\partial \zeta}\left[J\underbrace{\left(\frac{\partial \zeta}{\partial x}\sigma_{xx} + \frac{\partial \zeta}{\partial z}\sigma_{xz}\right)}_{\approx T_x}\right]\right\}$$



(Zhang and Chen, 2006; Zhang et al, 2012)

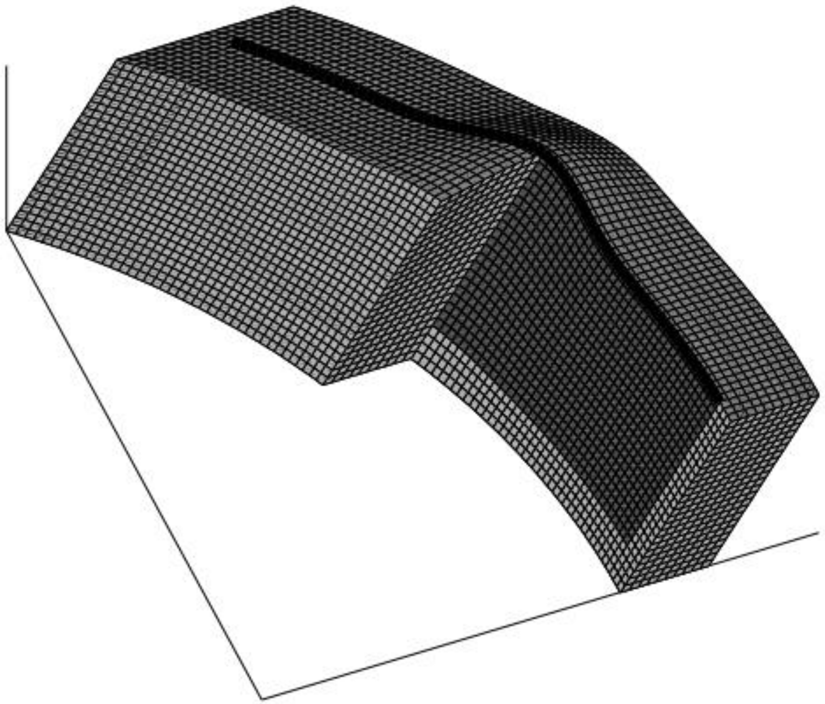
Smooth topography: vertical stretched grid

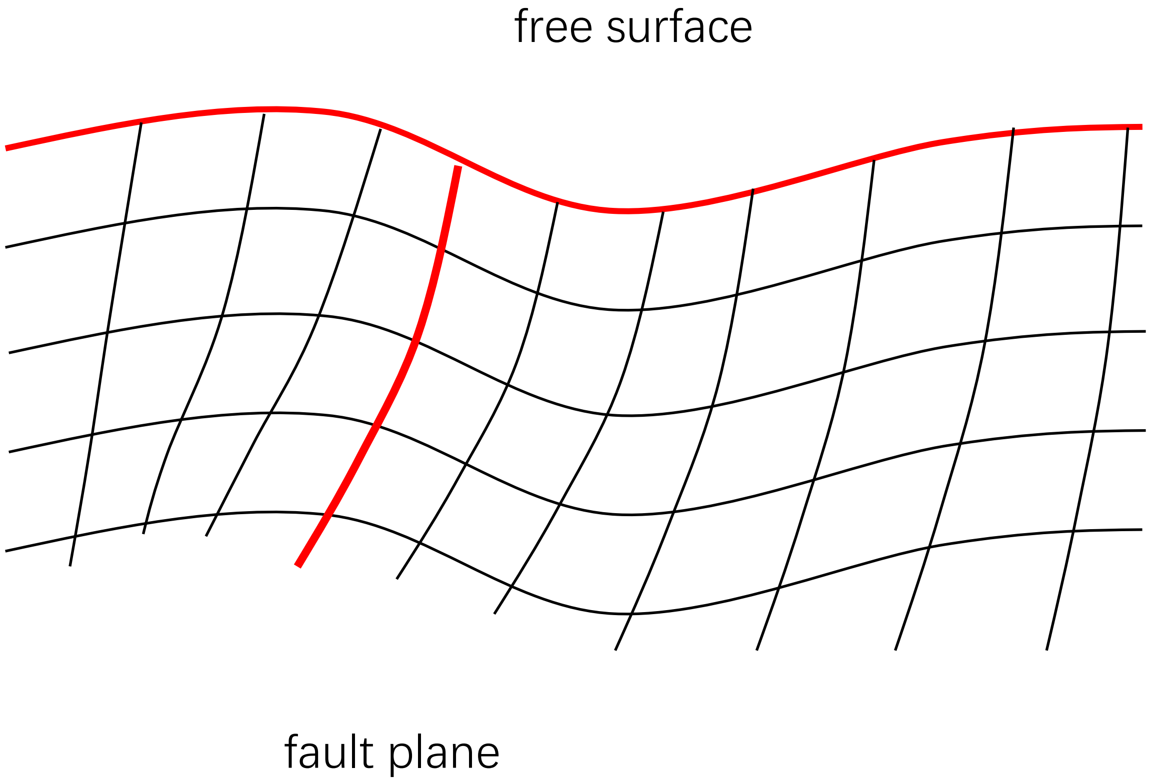


FDM： red line

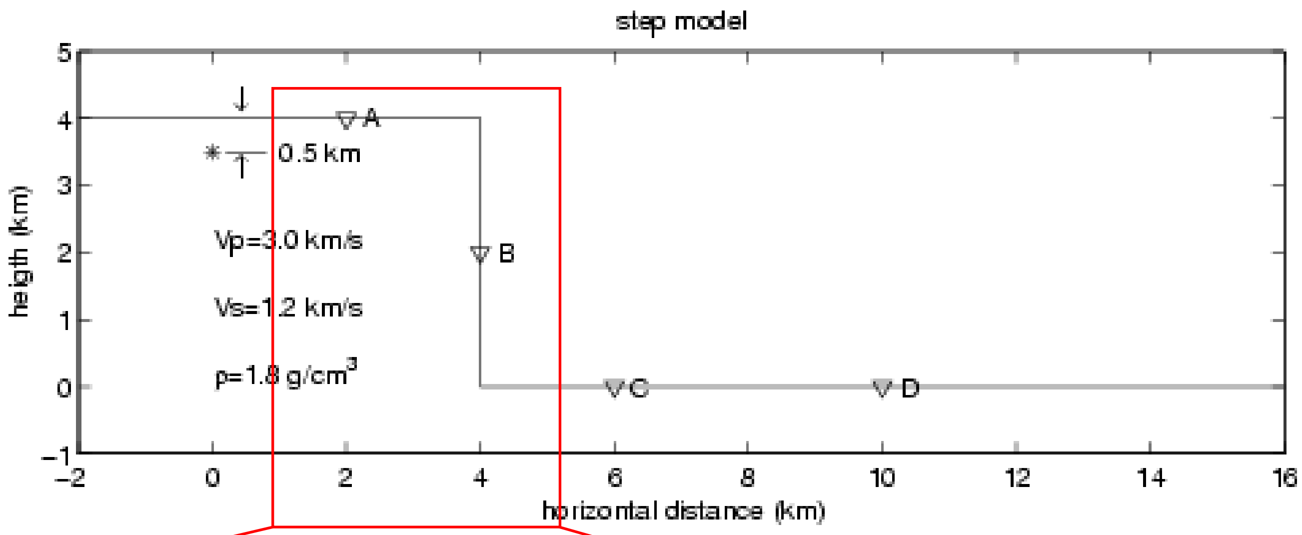
SEM： black line

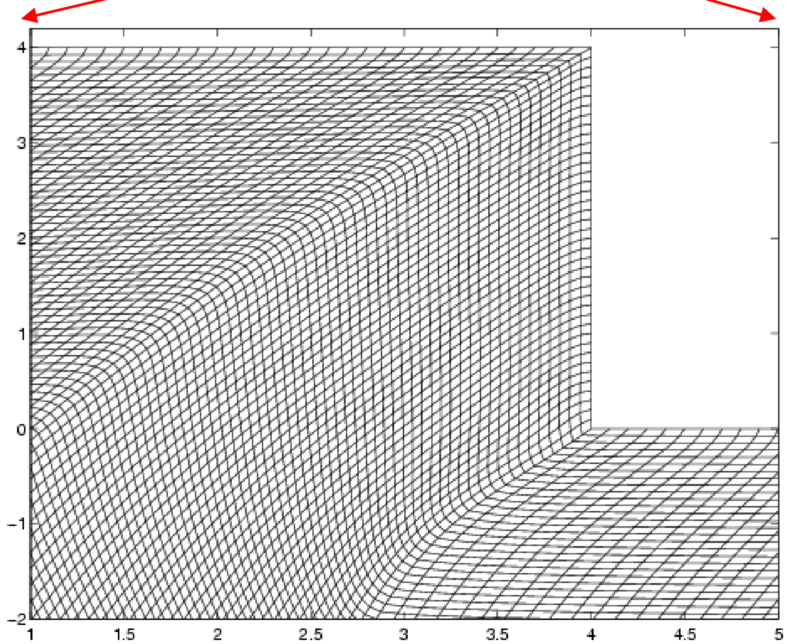
Topography+fault: general curvilinear grid

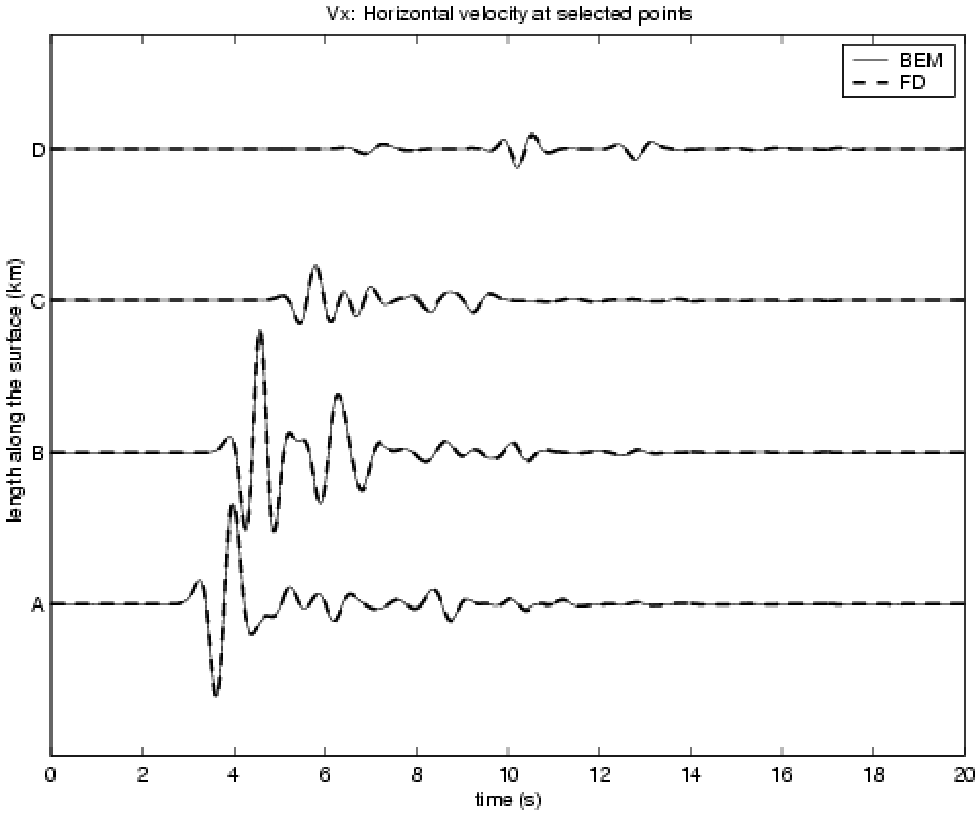




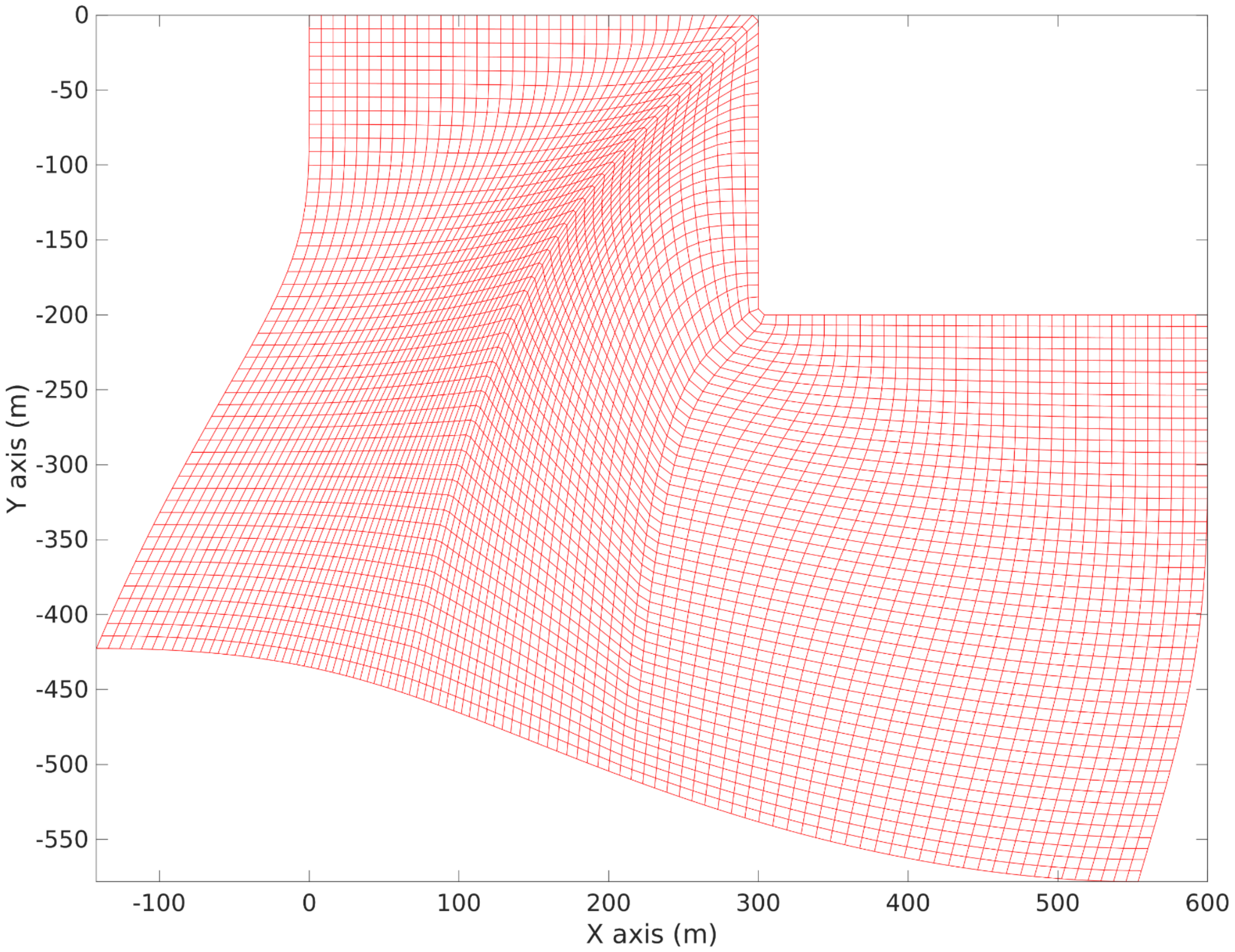
Rough topography: general curvilinear grid



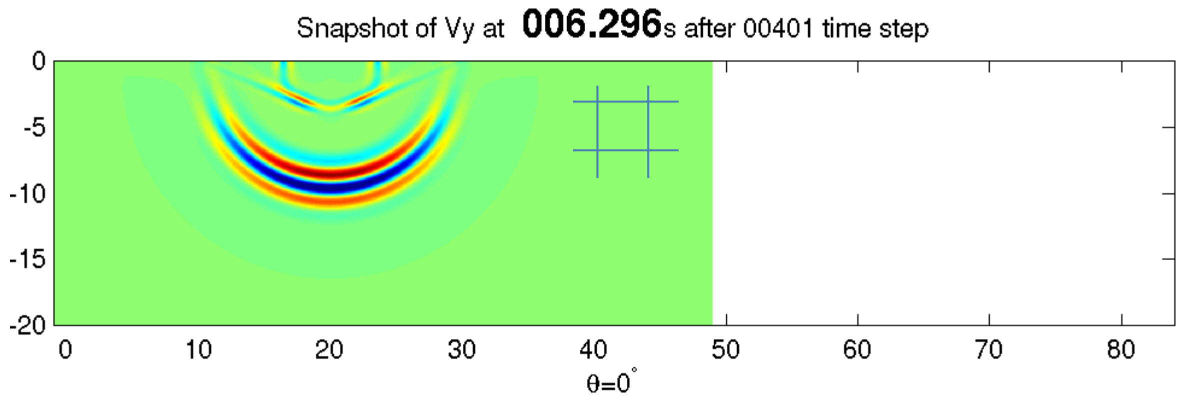




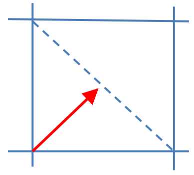
For seismic wave numerical simulation, only free surface is fixed, shapes of the other boundaries are free to be chosen



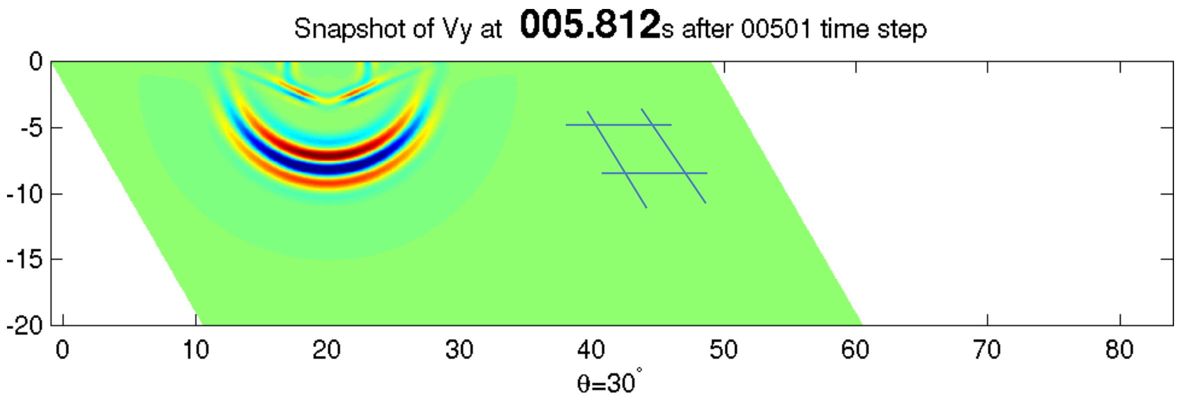
oblique grid does not affect accuracy, but reduce the time step of numerical stability



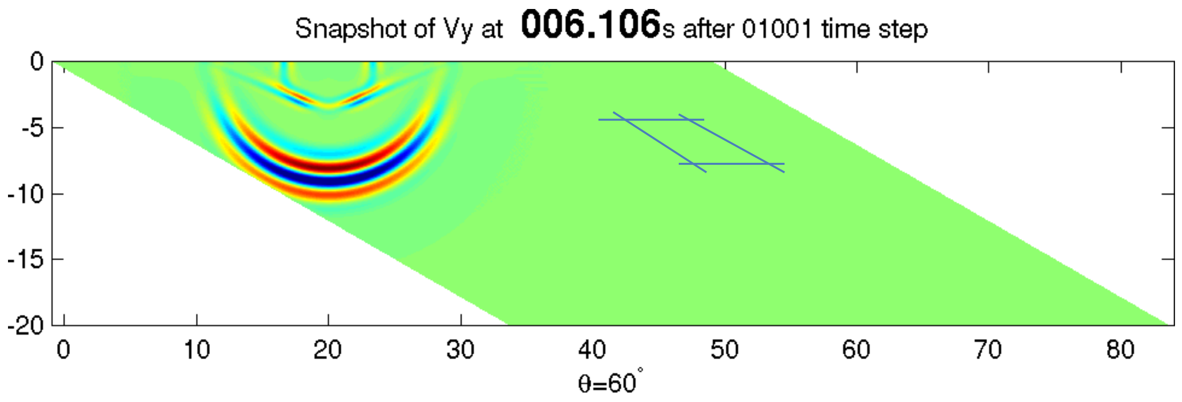
dt=0.015s



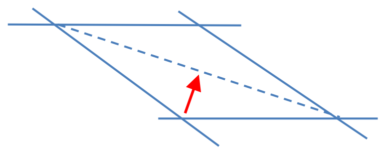
shortest propagation distance



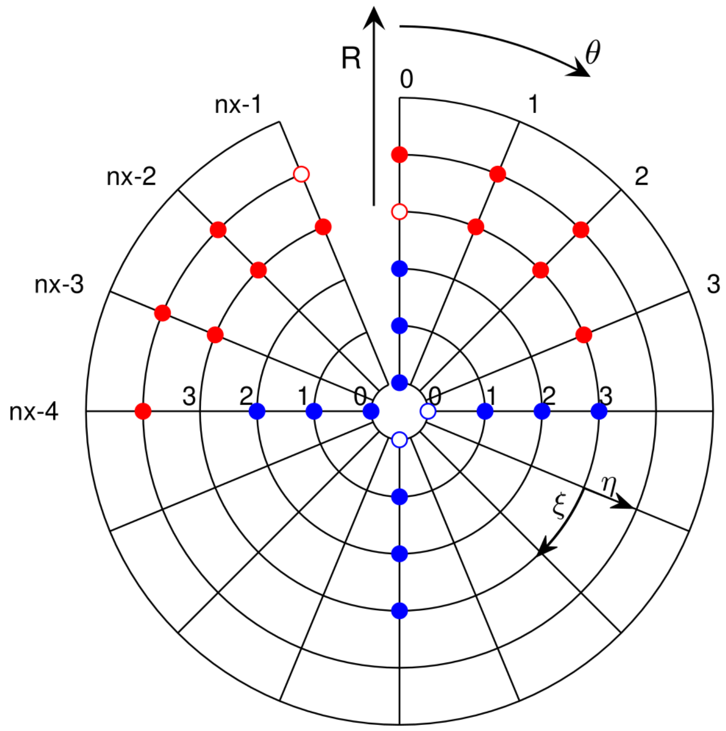
dt=0.011s



dt=0.006s



Global seismic waveform simulation (2D) with surface topography



physical coordinates of the grid

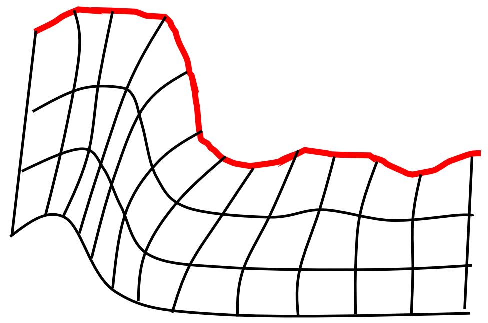
$$x(\xi,\eta) = R(\xi,\eta) * \sin(\theta(\xi)),$$

$$z(\xi,\eta) = R(\xi,\eta) * \cos(\theta(\xi)),$$

θis the longitude, R is the radius, which can vary with longitude

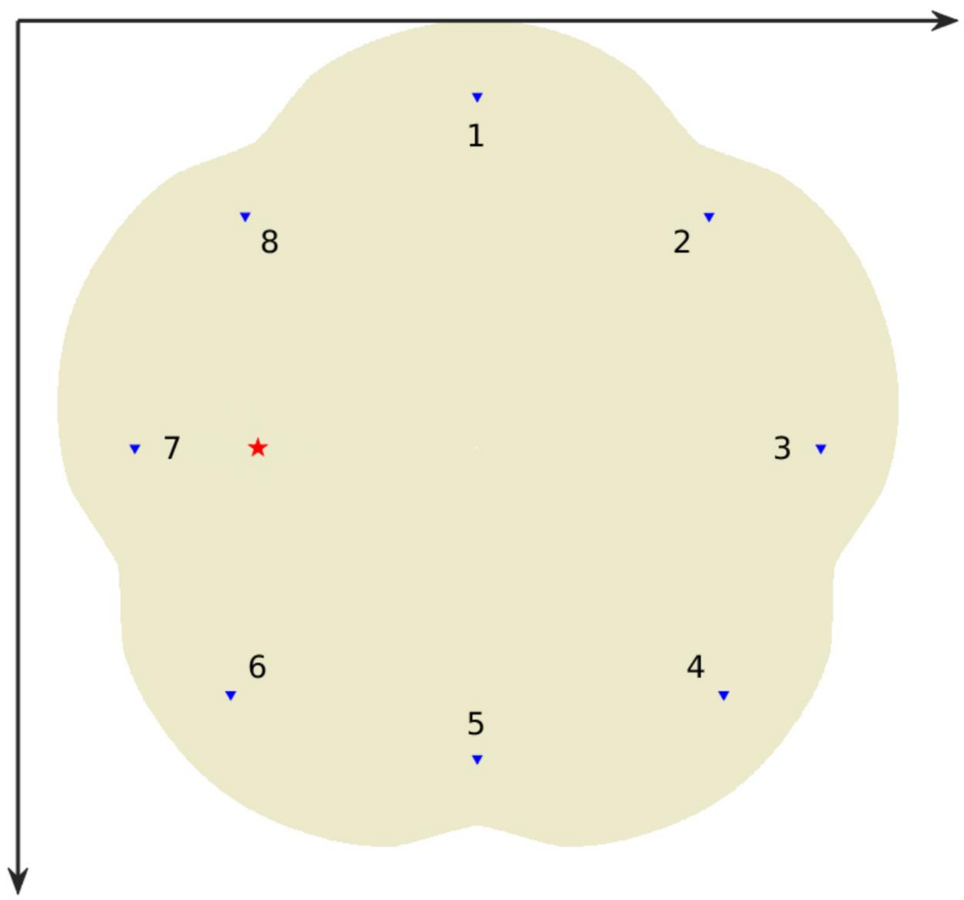
- variables are defined in global cartesian coordinate
- gradients are calculated in curvilinear coordinate
- input and output: polar coordinate

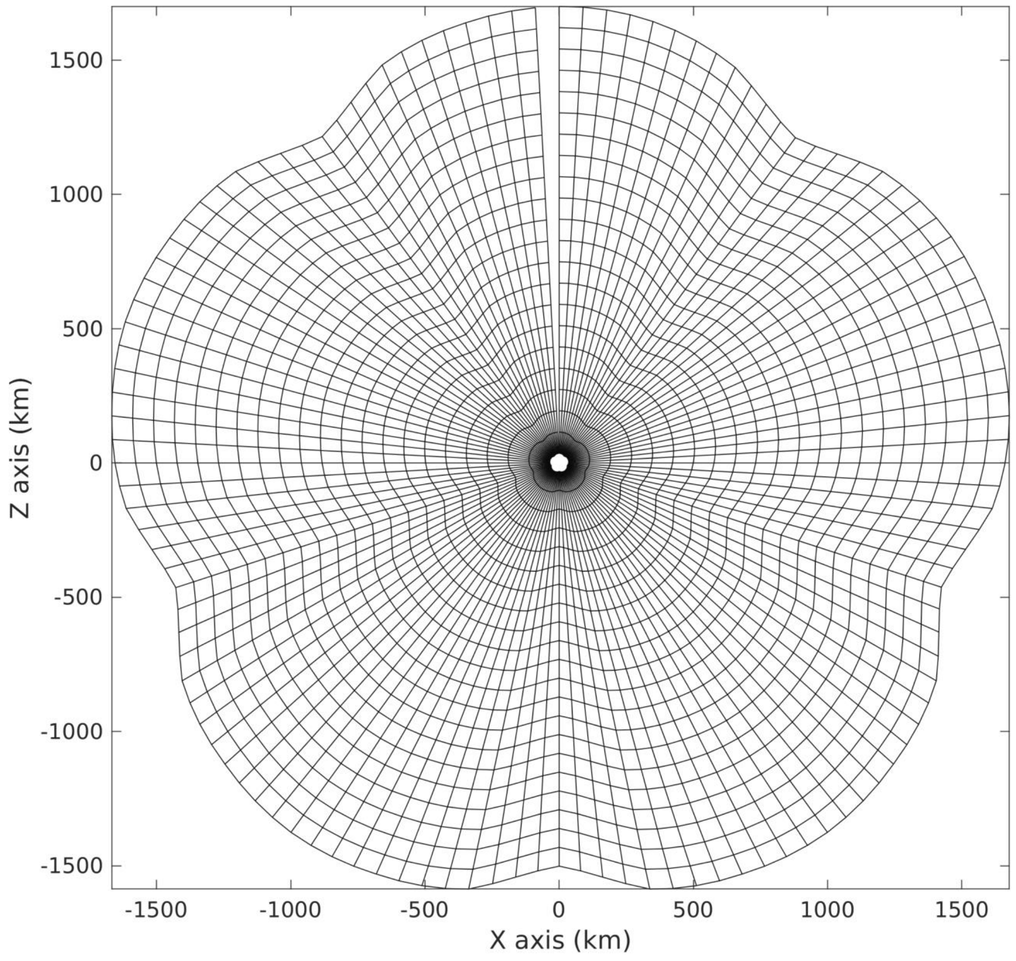
A special curvilinear grid



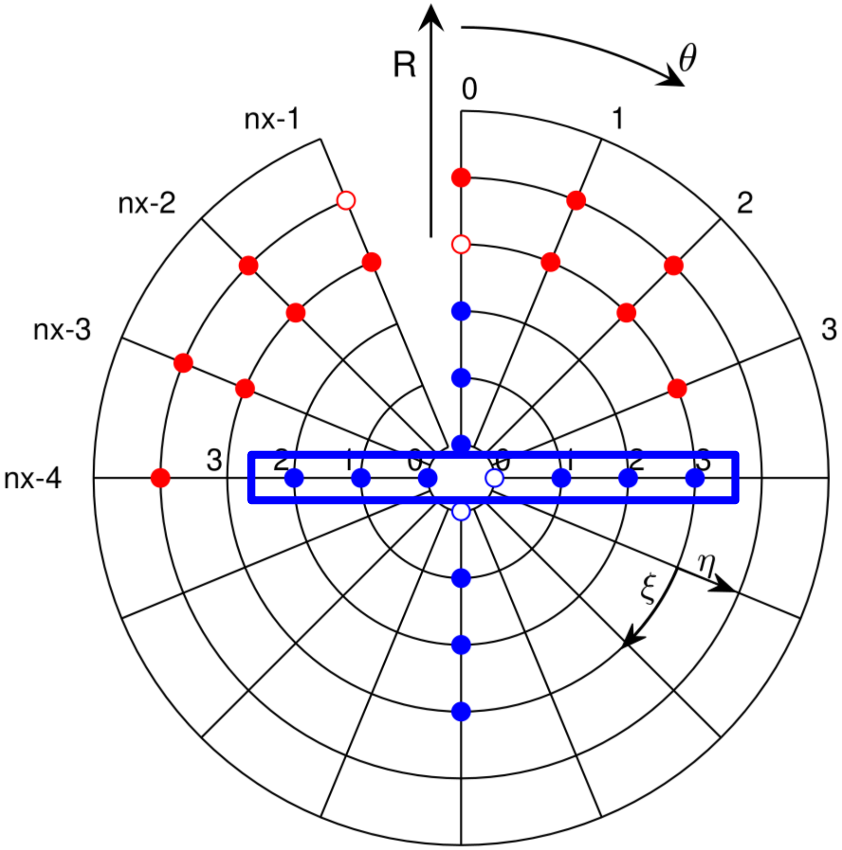
$$\rho \frac{\partial v_x}{\partial t} = \frac{\partial \xi}{\partial x}\frac{\partial \sigma_{xx}}{\partial \xi} + \frac{\partial \zeta}{\partial x}\frac{\partial \sigma_{xx}}{\partial \zeta} + \frac{\partial \xi}{\partial z}\frac{\partial \sigma_{xz}}{\partial \xi} + \frac{\partial \zeta}{\partial z}\frac{\partial \sigma_{xz}}{\partial \zeta}$$

Free surface topography can be taken into account

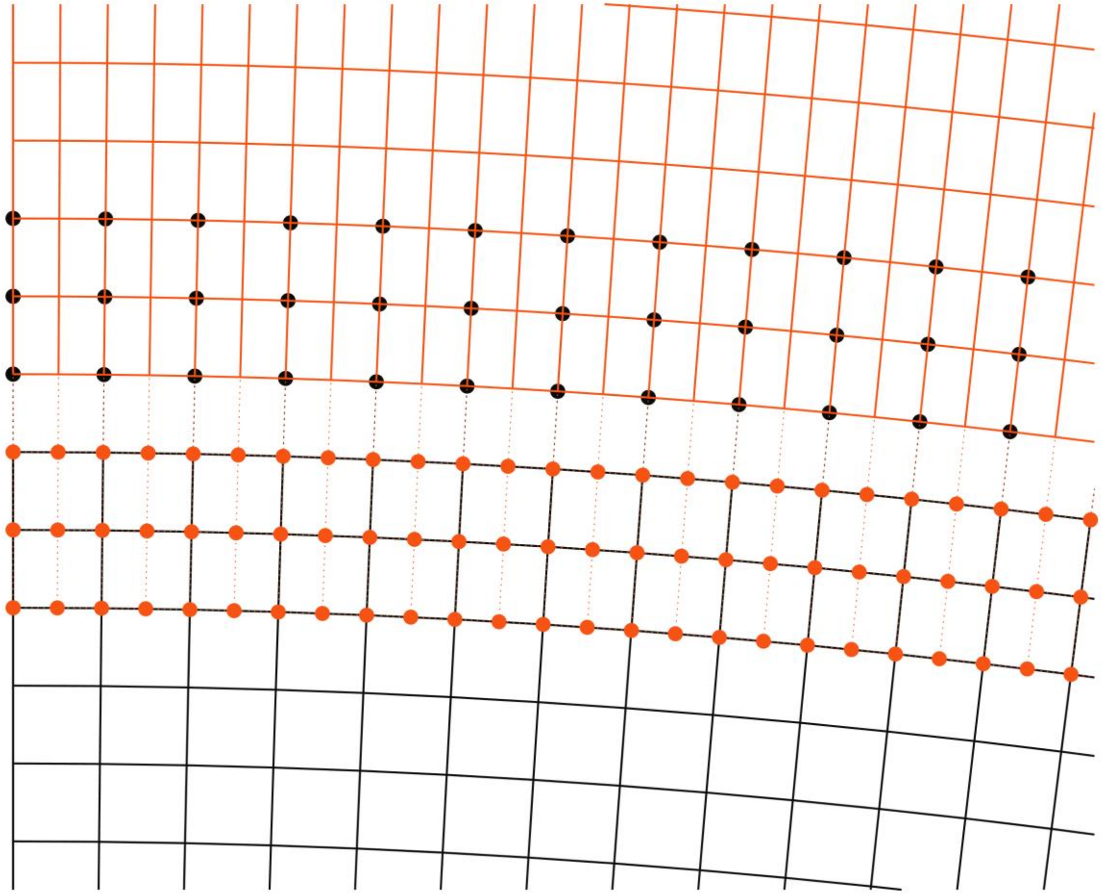




Do not define point at center

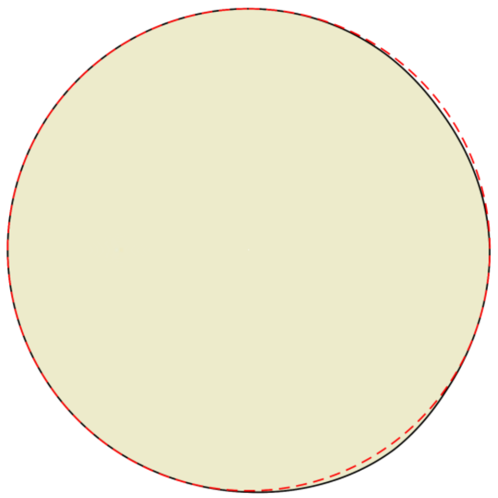


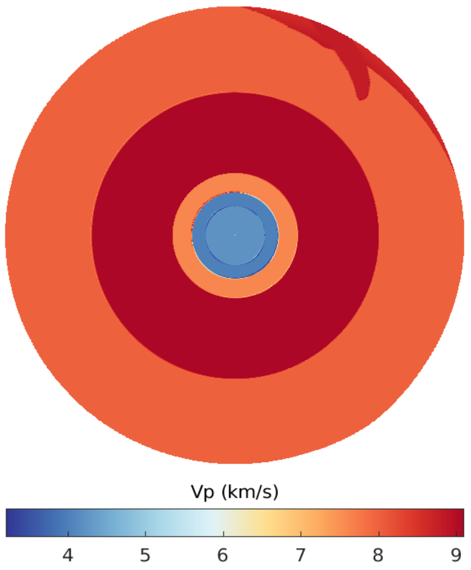
multi-level discontinues-grid

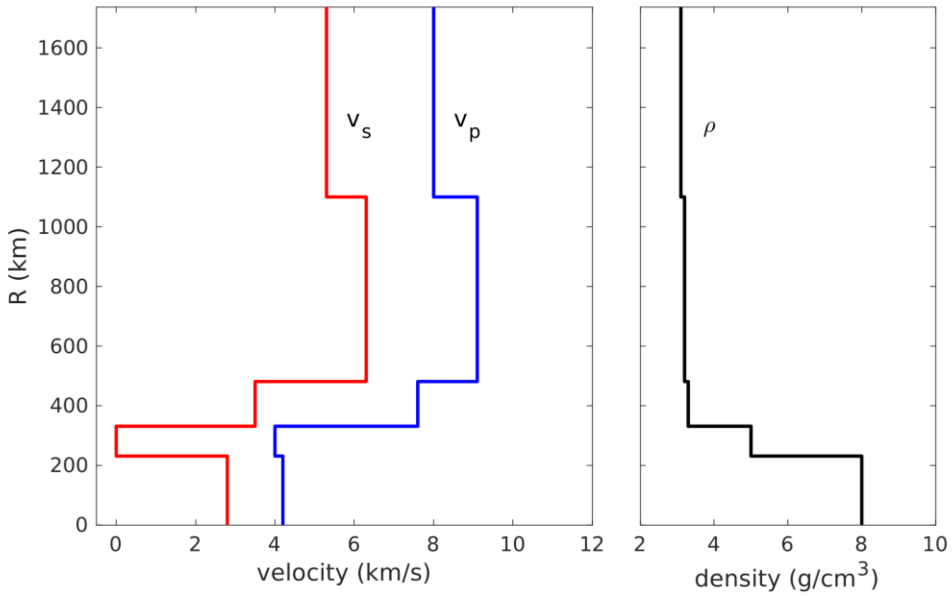


filter (Kristek et al., 2010; Zhang et al., 2013)
high-order interpolation

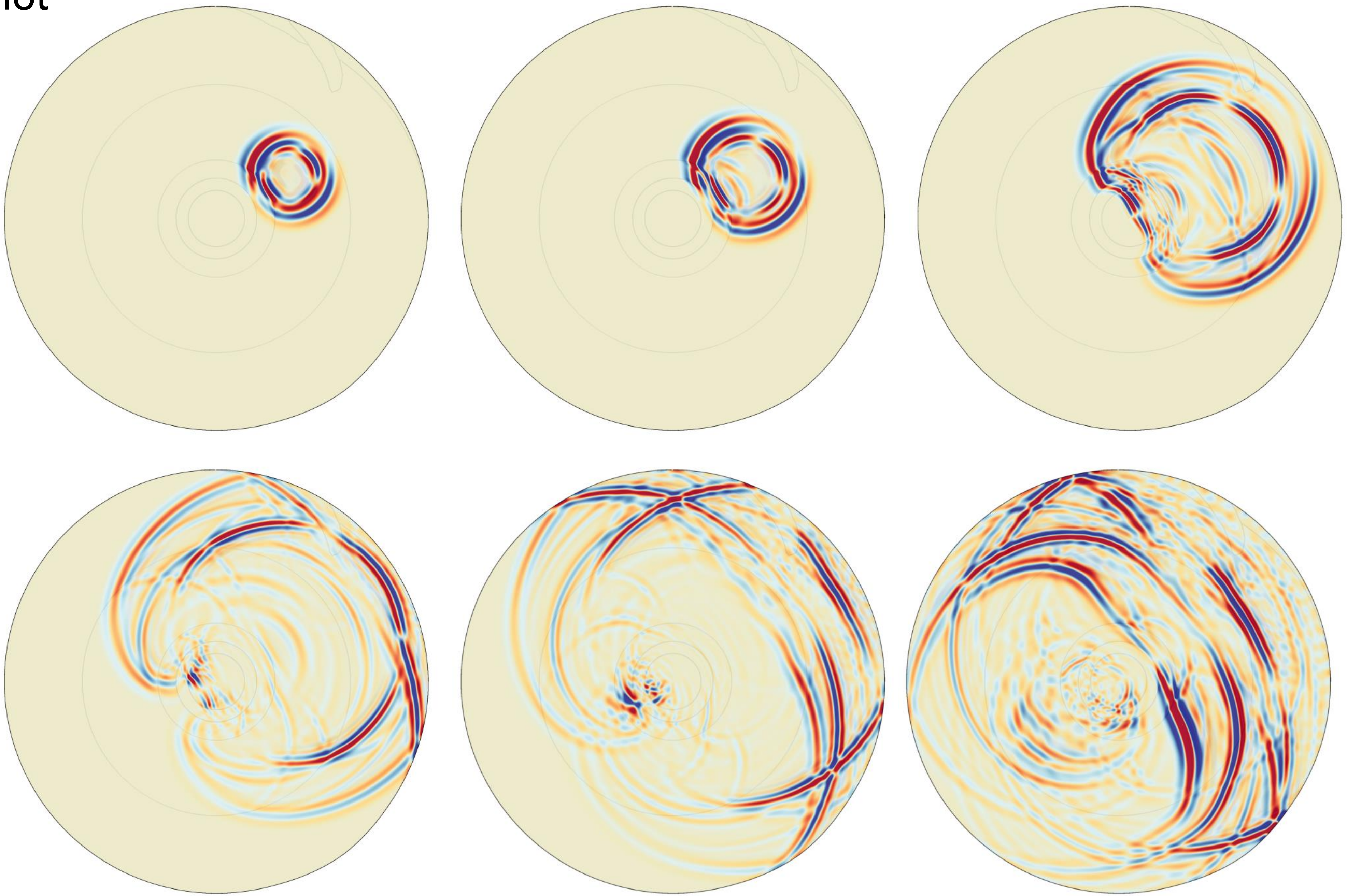
A simplified lunar model with high-speed anomalies and surface undulations







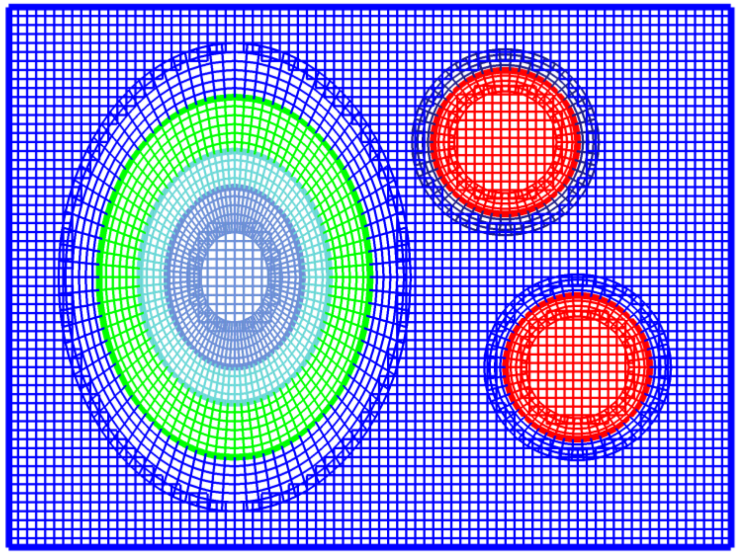
v_θ snapshot

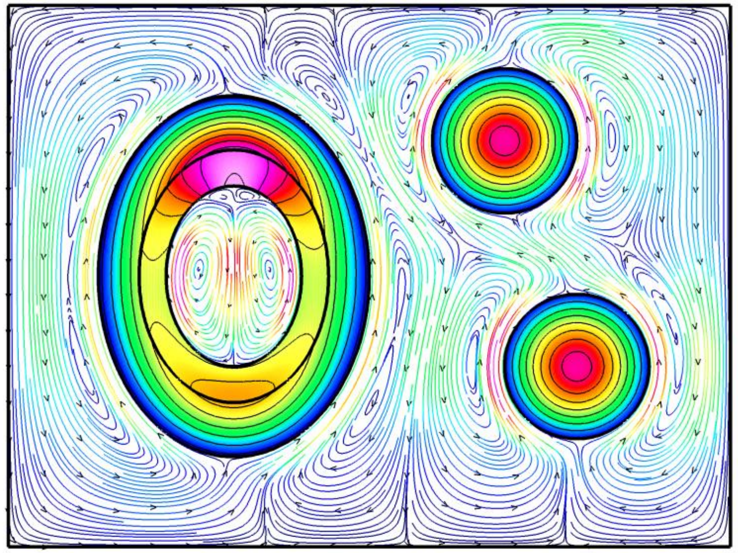


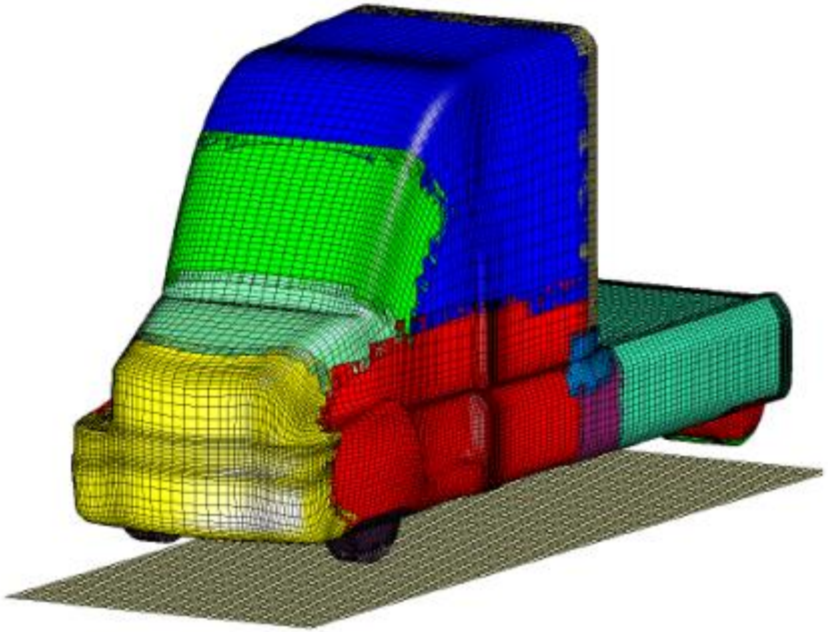
TOC

Complex geometries: overset grid / multiblock grid

Examples from computational Fluid Dynamics



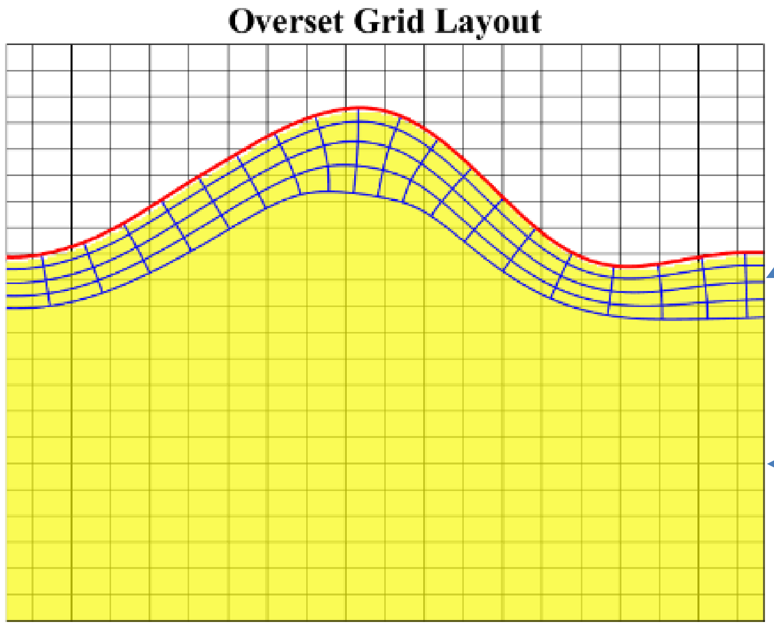




(Bill Henshaw, 2011)

- Update wavefield on each block
- use high-order interpolation to exchange messages between blocks (set values at ghost points)

Overset grid for rough topography

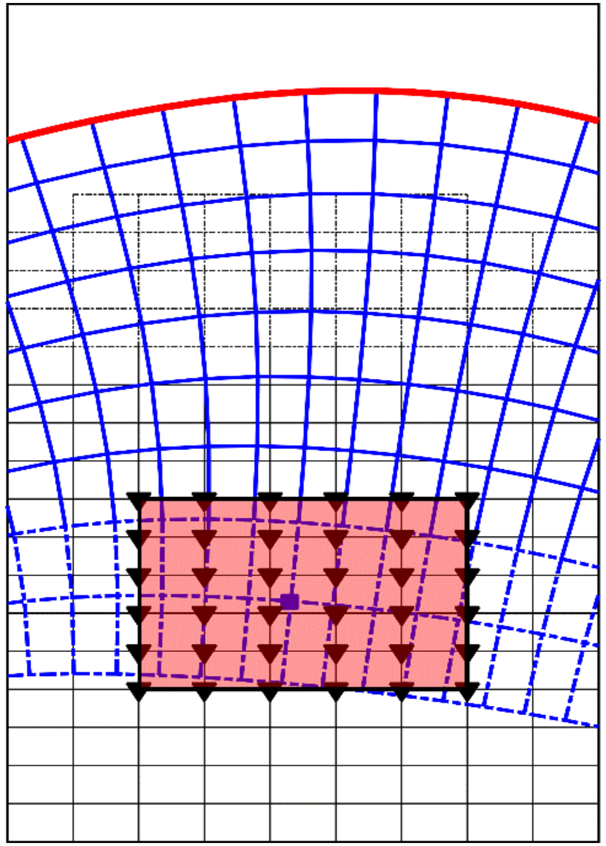


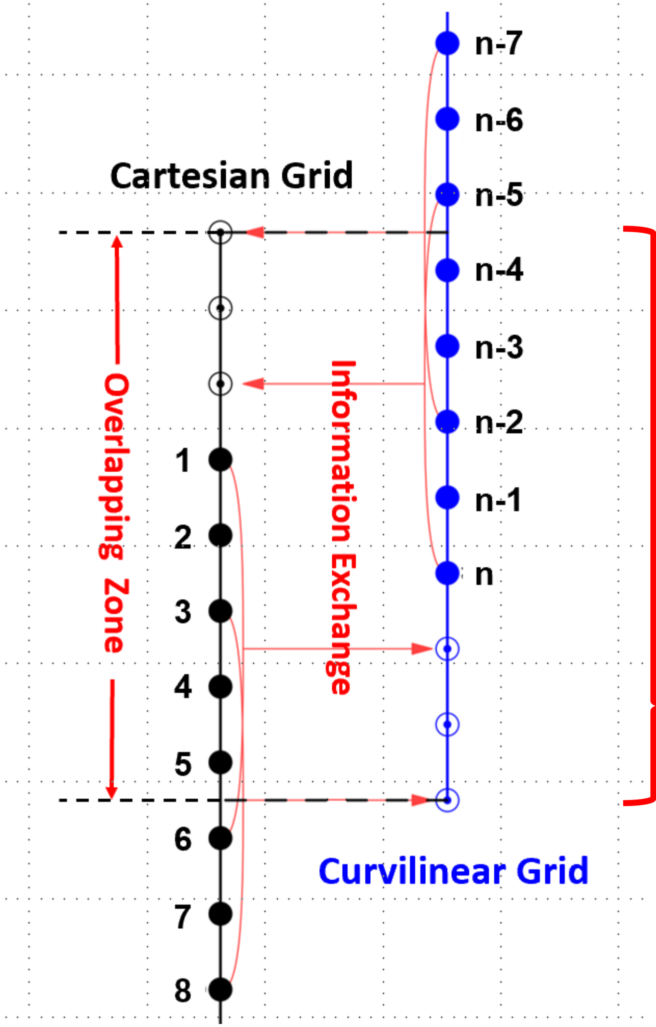
curvilinear grid near free surface

Cartesian grid covering whole region

- **reduce difficulty of grid generation:** fewer layers of curvilinear grid
- **improve computational efficiency:**
  - computing on Cartesian grids more efficient
  - near orthogonal curvilinear grid: increase step size

Nan Zang, Wei Zhang, and Xiaofei Chen, (2021), An overset-grid finite-difference algorithm for simulating elastic wave propagation in media with complex free-surface topography, GEOPHYSICS, 86(4):T277-T292





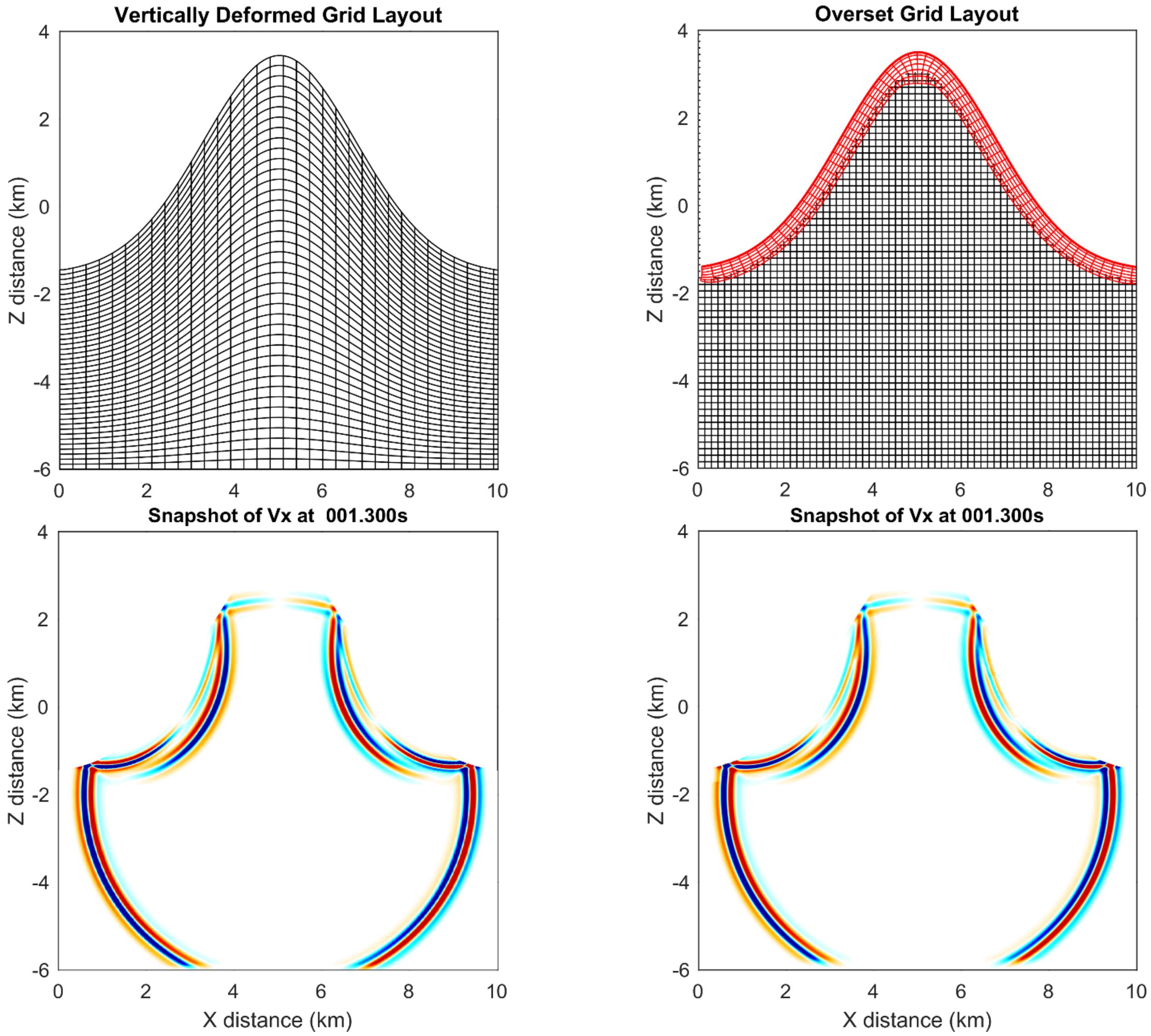
6th-order Lagrange interpolation

$$W_{target}(x_0, z_0) = \sum_{i=1}^{N=6} \sum_{j=1}^{N=6} L_{ij} W_{donor}(x_i, z_j)$$

$$L_{ij} = \prod_{l=1, l \neq i}^{N} \frac{x_0 - x_l}{x_i - x_l} \prod_{k=1, k \neq j}^{N} \frac{z_0 - z_k}{z_j - z_k}$$

5 interior points + 3 ghost points overlaid

A tall hill model



$\Delta t = 0.8ms$

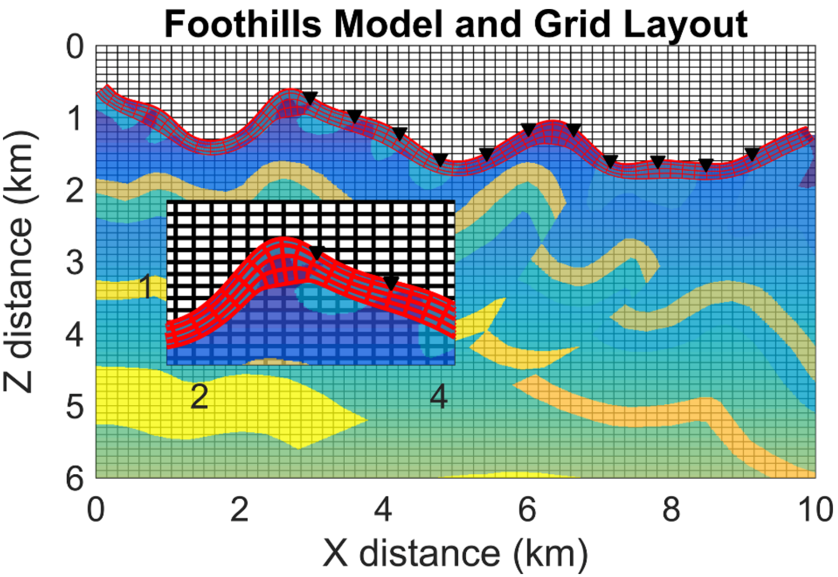
$\Delta t = 2.9ms$

3.6 times larger

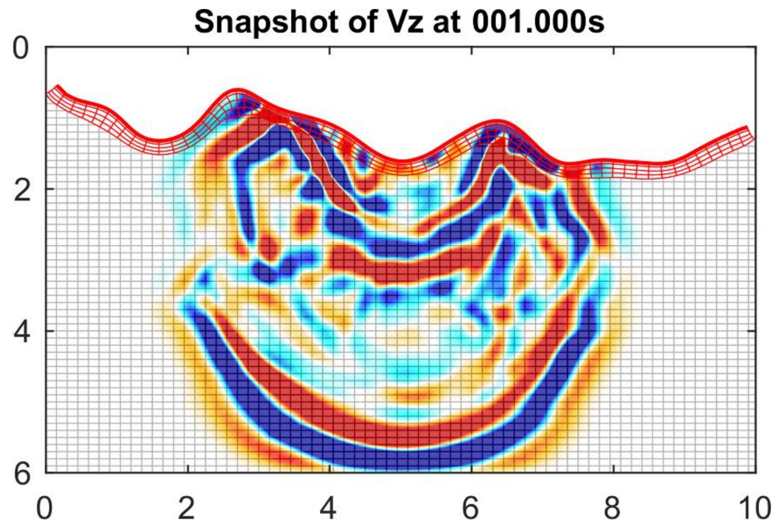
Max amplitude error: 2.65%

Max phase error: 0.65%

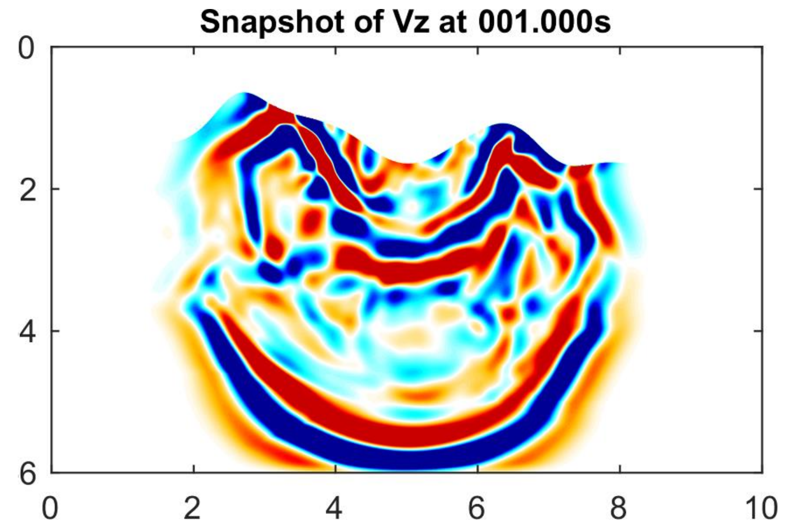
Complex velocity model：Foothills



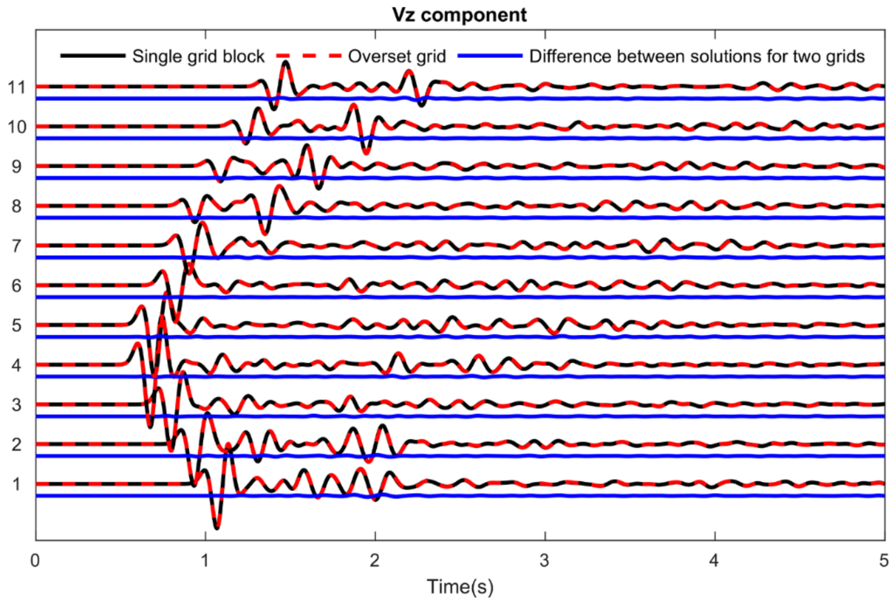
overset grid



single grid



- ☐ black color lines are the Cartesian grid
- ☐ red color lines are the curvilinear grid



amplitude error < 2.51%
phase error < 1.62%

Conclusions and Further Works

- Curvilinear grid FDM can simulate seismic wave propagation in models with complex boundary geometries
- Rough topography and whole Earth model with topography demonstrate the ability of the FDM to handle surface topography
- For very complex geometries, overset grid technique combining multiple cartesian and curvilinear grids is a standard and efficient solution for FDM

- Automatically generate 2D/3D curvilinear grid on the fly for large-scale simulation
- High-order free surface boundary condition implementation to reduce vertical PPW same to that of interior region

Thanks!