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# Parallel methods for wave modelling codes

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Code development main issues:

- Problem definition
- 📌 Hard- & Soft- Tools
- MATH representation
- GRID representation
- 💠 Examples



Problem definition

# Wave modelling for exploration geophysics engineering seismology







For realistic simulations:

heterogeneous properties must be correctly reproduced,

very complex structures
must be correctly modelled,

*numerical algorithms* must be computationally efficient. Space discretization:





### Geo-structure complexity



### Geo-structure heterogeneity





A huge computational effort,

both in memory storage
 (from Giga to Tera nodes),

& CPU time
 (from hours to weeks ).



Computational issues:

A highly accurate method is needed for reducing storage and CPU time requirements,

An efficient implementation of the algorithm is needed for reducing the total cost of the simulation.



## (consequences)

Algorithms must use:

\* vector/parallel platforms
(clusters, massive parallel...),

efficient hard-/soft-ware
 subroutines (FFT, Lapack, MPI...),

Iow count of operations & of primary storage (memory).

High-order methods:



## (possible choices)

# finite difference methods, pseudo-spectral methods, finite element methods, spectral element methods, finite volume methods, discontinous Galerkin methods.



# FD & Pseudo-spectral methods





### Matrix velocity-stress formulation

$$\frac{\partial}{\partial t}W = A \frac{\partial}{\partial x}W + B \frac{\partial}{\partial y}W + C \frac{\partial}{\partial z}W + f$$

$$W = \{v_x, v_y, v_z, \sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \sigma_{xy}, \sigma_{xz}, \sigma_{yz}\}^{\top}$$
$$f = \{f_x/\rho, f_y/\rho, f_z/\rho, 0, 0, 0, 0, 0, 0\}^{\top}$$
orcing source stress field  
particle velocity

## Matrices of elastic constants

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 $\lambda \& \mu$  Lame' elastic constants



 $\lambda \& \mu$  Lame' elastic constants



## $\lambda \& \mu$ Lame' elastic constants





Matrix velocity-stress formulation

$$\frac{\partial}{\partial t}W = A \tilde{D}_x W + B \tilde{D}_y W + C \tilde{D}_z W + f$$
  
Discrete space derivative operators

Computed by using:

Cartesían gríds





Matrix velocity-stress formulation

$$\frac{\partial}{\partial t}W = A \tilde{D}_x W + B \tilde{D}_y W + C \tilde{D}_z W + f$$
  
Discrete space derivative operators

Computed by using:

- Finite differences,
- Fourier Fast Transform,
- Chebyshev Fast Transform,
- Chebyshev Derivative Matrix.



Time integration is done by time stepping methods.

Can be obtained by differentiating an assumed expansion of the solution in given basis functions:

$$u(x) \approx u_N(x) = \sum_{j=0}^{N} \hat{u}_j \varphi_j(x)$$
 spectrul  
coefficients  
Basis functions

- Taylor expansion (finite differences),
- Trigonometric functions (pseudo-spectral periodic),
- Chebyshev or Legendre polynomials (pseudo-spectral).

Space derivative operators

Expressing the approximant with the values  $u_N(x_i)$ at the collocation points: node values

 $u_N(x) = \sum_{i=0}^N u_N(x_i) \phi_i(x)$ 

Lagrange or cardinal basis

$$\partial_x u_N(x) = \sum_{i=0}^N u_N(x_i) \; \partial_x \phi_i(x) = \sum_{i=0}^N u'_N(x_i) \; \phi_i(x)$$

$$u'_{N}(x_{i}) = \sum_{j=0}^{N} (\tilde{\mathbf{D}}_{x})_{ij} \ u_{N}(x_{j}) \quad \longleftrightarrow \quad U'_{N} = \tilde{\mathbf{D}}_{x} \ U_{N}$$

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Finite difference methods:

- banded matrix derivatives,
- efficient code implementation,
- low order & accuracy rely on order.

Pseudo-spectral methods:

- full matrix derivatives,
- efficient code implementation using FFT,
- high order & high accuracy.

## Parallel computation Pseudo-spectral methods





## Parallel computation Pseudo-spectral methods





**Global communications** 

## Parallel computation Multi-Domain Block Decomposition

### MDBD pseudo-spectral method:

- - \* Blocks decomposed in small overlapping
    elements ,
- Derivatives computed concurrently in each element by the Chebyshev pseudo-spectral method,
- Continuity across the element boundaries assured by the overlap of the discrete derivative operator,
- Same accuracy order at interfaces & in elements.







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Chebyshev Derivative & Overlap



Given  $\mathbf{A} = [a_{ij}]^{m \times n}$  &  $\mathbf{B} = [b_{ij}]^{p \times q}$ 

 $\mathbf{A} \otimes \mathbf{B} \doteq \begin{bmatrix} a_{11}\mathbf{B} & a_{12}\mathbf{B} & \dots & a_{1n}\mathbf{B} \\ a_{21}\mathbf{B} & a_{22}\mathbf{B} & \dots & a_{2n}\mathbf{B} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1}\mathbf{B} & a_{m2}\mathbf{B} & \dots & a_{mn}\mathbf{B} \end{bmatrix} \begin{array}{c} \text{block matrix} \\ \text{of order} \\ (\text{mp x nq}) \end{array}$ 

Vec  $(\bullet)$ 

reshapes a generic rank-K tensor in a column vector of length

 $n_1 n_2 \cdots n_K$ 



• Generalized inner product:

$$\mathbf{A} \star \mathbf{U} \doteq \sum_{l=0}^{N} A_{il} U_{lmn}$$
  
Generalized transpose:  
$$(U_{ijk})^{\top} \doteq U_{jki}$$

by Kronecker product properties

 $(\mathbf{A}^e \otimes \mathbf{B}^e \otimes \mathbf{C}^e) \operatorname{Vec}(U^e) =$ 

 $Vec(\mathbf{A}^{e} \star (\mathbf{B}^{e} \star (\mathbf{C}^{e} \star U^{e})^{\top})^{\top})^{\top})$ 

# Derivative by Kronecker Product

- $ilde{\mathbf{D}}^e_x = \mathbf{I}^e_z \otimes \mathbf{I}^e_y \otimes \mathbf{D}^e_x$
- $ilde{\mathbf{D}}_y^e = \mathbf{I}_z^e \otimes \mathbf{D}_y^e \otimes \mathbf{I}_x^e$
- $ilde{\mathbf{D}}^e_z = \mathbf{D}^e_z \otimes \mathbf{I}^e_y \otimes \mathbf{I}^e_x$

3D Pseudo-spectral element derivative operators

Unity matrix

by Kronecker product properties

- $\tilde{\mathbf{D}}_x^e(U^e) = (\mathbf{I}_z^e \star (\mathbf{I}_y^e \star (\mathbf{D}_x^e \star U^e)^\top)^\top)^\top \qquad \mathbf{X} axis$
- $\tilde{\mathbf{D}}_{y}^{e}(U^{e}) = (\mathbf{I}_{z}^{e} \star (\mathbf{D}_{y}^{e} \star (\mathbf{I}_{x}^{e} \star U^{e})^{\top})^{\top})^{\top} \qquad \mathbf{Y} \mathbf{axis}$
- $\tilde{\mathbf{D}}_{z}^{e}(U^{e}) = (\mathbf{D}_{z}^{e} \star (\mathbf{I}_{y}^{e} \star (\mathbf{I}_{x}^{e} \star U^{e})^{\top})^{\top})^{\top} \qquad \mathbf{Z} \text{-axis}$

# Derivative by Kronecker Product

Element wave field:

$$U_{ijk}^{e} = u^{e}(x_{i}, y_{j}, z_{k}, t) = Vec (U^{e})_{k\bar{N}^{2}+j\bar{N}+i+1}$$
  
grid values  
interbolation order N

N = N + 1

Pseudo-spectral element derivatives:

$$\begin{split} \tilde{\mathbf{D}}_{x}^{e}(U^{e}) &= \mathbf{D}_{x}^{e} \star U^{e} & \mathsf{X} \text{ - axis} \\ \tilde{\mathbf{D}}_{y}^{e}(U^{e}) &= (\mathbf{D}_{y}^{e} \star U^{e^{\top}})^{\top \top} & \mathsf{Y} \text{ - axis} \\ \tilde{\mathbf{D}}_{z}^{e}(U^{e}) &= (\mathbf{D}_{z}^{e} \star U^{e^{\top} \top})^{\top} & \mathsf{Z} \text{ - axis} \end{split}$$

Computed by optimized *matrix-matrix* products (LAPACK)

Synchronization & communications



MDBD Scaled // Speed-up



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Number of Processors

MDBD Scaled // Speed-up

J.OGS

32800 elements

9 nodes/element

419400 elements 45.1 Gw (1796x898x898)





# Spherical Coordinates



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# Cubed Sphere











# Finite element methods (FEM) & Spectral element methods (SEM)



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$$\rho \frac{\partial^2 \boldsymbol{u}}{\partial t^2} - \nabla [(\lambda + 2\mu) \nabla \cdot \boldsymbol{u}] - \nabla \cdot (\mu \nabla \boldsymbol{u}) = \mathbf{f}$$

$$\rho \frac{\partial^2 \boldsymbol{u}}{\partial t^2} - \mathcal{D}^\top \boldsymbol{\sigma} = \mathbf{f}$$

matrix formulation

 $\sigma(u) = C \epsilon(u)$  stress-strain relation

 $\epsilon(u) = \mathcal{D} u$  strain-displacement relation

2D elastic wave equation



$$\rho \frac{\partial^2 \boldsymbol{u}}{\partial t^2} - \mathcal{D}^{\top} \boldsymbol{\sigma} = \mathbf{f}$$

in 2D:

$$\mathcal{D} = \begin{bmatrix} \partial_x & 0 \\ 0 & \partial_y \\ \partial_y & \partial_x \end{bmatrix}$$

### differential operator

$$oldsymbol{C} \;=\; \left[ egin{array}{ccc} \lambda+2\mu & \lambda & 0 \ \lambda & \lambda+2\mu & 0 \ 0 & 0 & \mu \end{array} 
ight]$$

### elastic stiffness matrix

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}(\boldsymbol{x}, t) = \{\sigma_{xx}, \ \sigma_{yy}, \ \sigma_{xy}\}\$$
$$\boldsymbol{\epsilon} = \boldsymbol{\epsilon}(\boldsymbol{x}, t) = \{\epsilon_{xx}, \ \epsilon_{yy}, \ \epsilon_{xy}\}^{\top}$$

stress & strain vectors







$$ho rac{\partial^2 oldsymbol{u}}{\partial t^2} - \mathcal{D}^{ op} oldsymbol{\sigma} = \mathbf{f}$$
 strong form

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$$\frac{d^2}{dt^2} \int_{\Omega} \rho \, \boldsymbol{w}^{\top} \boldsymbol{u} \, d\Omega + \int_{\Omega} \boldsymbol{w}^{\top} \mathcal{D}^{\top} \mathbf{C} \, \mathcal{D} \, \boldsymbol{u} \, d\Omega = \int_{\Omega} \boldsymbol{w}^{\top} \mathbf{f} \, d\Omega$$





$$\rho \frac{\partial^2 \boldsymbol{u}}{\partial t^2} - \mathcal{D}^{\top} \boldsymbol{\sigma} = \mathbf{f}$$
 weak form  
$$\frac{d^2}{dt^2} \int_{\Omega} \rho \, \boldsymbol{w}^{\top} \boldsymbol{u} \, d\Omega + \int_{\Omega} \boldsymbol{w}^{\top} \mathcal{D}^{\top} \mathbf{C} \, \mathcal{D} \, \boldsymbol{u} \, d\Omega = \int_{\Omega} \boldsymbol{w}^{\top} \mathbf{f} \, d\Omega$$



$$\rho \frac{\partial^2 \boldsymbol{u}}{\partial t^2} - \mathcal{D}^\top \boldsymbol{\sigma} = \mathbf{f}$$

$$\frac{d^2}{dt^2} \int_{\Omega} \rho \, \boldsymbol{w}^{\top} \boldsymbol{u} \, d\Omega \, + \, \int_{\Omega} \boldsymbol{w}^{\top} \mathcal{D}^{\top} \mathbf{C} \, \mathcal{D} \, \boldsymbol{u} \, d\Omega \, = \, \int_{\Omega} \boldsymbol{w}^{\top} \mathbf{f} \, d\Omega$$
$$\tilde{\boldsymbol{u}}^e(x, y, z, t) \, = \, \sum_{i, j, k=0}^{N} \boldsymbol{u}^e_{ijk}(t) \, \Phi_{ijk}(x, y, z)$$
$$\mathbf{M} \, \ddot{\boldsymbol{U}} \, + \, \mathbf{K} \, \boldsymbol{U} \, = \, \boldsymbol{F}$$

Solve a system of second order ordinary differential equations



$$\rho \frac{\partial^2 \boldsymbol{u}}{\partial t^2} - \mathcal{D}^\top \boldsymbol{\sigma} = \mathbf{f}$$

$$\frac{d^2}{dt^2} \int_{\Omega} \rho \, \boldsymbol{w}^{\top} \boldsymbol{u} \, d\Omega + \int_{\Omega} \boldsymbol{w}^{\top} \mathcal{D}^{\top} \mathbf{C} \, \mathcal{D} \, \boldsymbol{u} \, d\Omega = \int_{\Omega} \boldsymbol{w}^{\top} \mathbf{f} \, d\Omega$$



Solve a system of second order ordinary differential equations



ρ

 $\mathbf{M}$ 

$$rac{\partial^2 oldsymbol{u}}{\partial t^2} ~-~ \mathcal{D}^ op oldsymbol{\sigma} = \mathbf{f}$$

$$\frac{d^2}{dt^2} \int_{\Omega} \rho \, \boldsymbol{w}^{\top} \boldsymbol{u} \, d\Omega \, + \, \int_{\Omega} \boldsymbol{w}^{\top} \boldsymbol{\mathcal{D}}^{\top} \mathbf{C} \, \boldsymbol{\mathcal{D}} \, \boldsymbol{u} \, d\Omega \, = \, \int_{\Omega} \boldsymbol{w}^{\top} \mathbf{f} \, d\Omega$$

$$\ddot{m{U}}$$
 + K $m{U}$  = F  
 $\dot{m{U}}(0)$  =  $m{U}_0$   
 $\dot{m{U}}(0)$  =  $\dot{m{U}}_0$ 

Solve a system of second order ordinary differential equations



### Finite elements:

- Iow order & low accuracy (in general),
- shape functions by linear, quadratic and cubic polynomials,
- triangular/quadrangular or tetrahedral/hexahedral elements.

### Spectral elements:

- high order & high accuracy,
- shape functions by Chebyshev and Legendre orthogonal polynomials,
- quadrangular or hexahedral elements.

## SEM in 3D: Mesh design

#### Realistic example: The Grenoble valley



# LOGS

### Chebyshev polynomials:

- non-diagonal system matrices,
- implicit schemes(in time) => linear systems solution
  (fast solvers, sub-structuring/EBE-iterative),
- unconditionally stable => large time steps.

### Legendre polynomials:

- diagonal system matrices,
- \* explicit schemes(in time) => faster (in principle),
- conditionally stable => time steps must honour CFL limit.

## Parallel computation SEM methods



### Domain partition



# SEM partitioning



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### Modeling of Scattered Waves in Merapi Volcano

(J. Wassermann)



problem adapted mesh generation
load balancing by partitioning & grouping subdomains (see Metis or Jostle software)





Parallel implementation

Very efficient parallel codes can be developed because in solving:

$$\mathbf{M}\ \ddot{\boldsymbol{U}}\ +\ \mathbf{K}\ \boldsymbol{U}\ =\ \boldsymbol{F}$$

- \* most of calculation are based on linear algebra op.,
- Interpretation of the second state of the s
- slobal matrix-vector products can be easily computed at element level and back:

$$\mathbf{v} = \mathbf{S} \mathbf{p} \iff \mathbf{v}^{(e)} = \mathbf{S}^{(e)}\mathbf{p}^{(e)}$$

 element level op. can be done element-by-element (EBE) in any order or in parallel. EBE algorithm

Parallel implementation

DO in parallel:

- gather data from global to local
- Iocal matrix-vector multiply
- \* scatter data from local to global  $\mathbf{v}^{(e)} \Longrightarrow \mathbf{v}$ ,
- \* synchronize data at subdomain interfaces by MPI call.

**REPEAT** for each step.





 $\mathbf{p} \implies \mathbf{p}^{(e)}$ 

 $\mathbf{v}(e) = \mathbf{S}(e)\mathbf{p}(e) ,$ 



Global seismology



### SPECFEM3D

### (D. Komatitsch, J. Tromp et al.)





New machine:

- 512 dual-processor quad-core nodes (4096 cores)
- 6 TB of distributed memory
- 22.6 TFLOPS
- Half the cooling & power

- "Old" machine:
- 1024 nodes/2048 processors
- 3 TB of distributed memory
- 13.1 TFLOPS

## Global seismology



### SPECFEM3D

### (D. Komatitsch, J. Tromp et al.)

## **Spectral-Element Method**

- Flexibility of the finite-element method •
- Accuracy of a pseudospectral method ٠
- Gauss-Lobatto-Legendre (GLL) quadrature •
- Lagrange interpolants ٠
- **Diagonal mass matrix**
- Explicit time integration  $\bullet$





#### Lagrange polynomials



Omar Ghattas (UT Austin), T. Tu, H. Yu (CMU)

- Avoid scalability bottlenecks (serial algorithms, file I/O)
- Integrate meshing, partitioning, simulation and visualization in a single parallel end-to-end application
- All operations are done in parallel and in-core (no I/O)
- Online remote steering of the parallel process by GUI



Octree-based scalable adaptive fe

Prospects for Seismic Inversion On Petaflop Systems  $\rightarrow$  This talk is about parallel computing.

Kilo – 1,000 Mega – 1,000,000 Giga – 1,000,000,000 Tera – 1,000,000,000,000 Peta – 1,000,000,000,000,000

Flop – "Floating Point Operation"

Example Earthquake Simulation:

- 600km x 600km x 70km region
- Average velocity 2km/s, Max frequency 2Hz
- Wavelength 1km
- 10 variables per wavelength 25 billion variables
- Simulated waves travel 400km 4000 time steps
- Executing on average 10 arithmetic operations per variable

- 25 million grid boxes



# Examples



Acquansanta viaduct





## Acquansanta viaduct





## Acquansanta viaduet





## Acquansanta viaduet







Thank for your attention!

ICTP School for HPC applications in Earth Sciences, November 2014, Trieste