### Progress and Challenges in Computational Geodynamics

Marc Spiegelman (Columbia/LDEO)

# Lecture I: Overview of Computational Geodynamics Computational Seismology

© 2010 Google © 2010 Tele Atlas © 2010 Europa Technologies US Dept of State Geographer

©20

### Overview of Lectures

- Lecture 1: The Context: Plate Tectonics and Computational Seismology
- Lecture II: Solid Mechanics Mantle Convection/ Lithospheric Deformation/Earthquake Physics
- Lecture III: Magma Dynamics coupled fluid-solid problems
- Lecture IV: Putting it all together, toward a consistent computational framework for complex multi-physics problems

© 2010 Google © 2010 Tele Atlas © 2010 Europa Technologies US Dept of State Geographer

### Lecture

Introduction to Solid Earth Geoscience: Plate Tectonics 101 **Overview of Computational Geodynamics Computational Seismology** The Forward Problem Math, Methods, performance The Inverse Problem ( Available Software: the SPECFem family of HP © 2010 Google codes © 2010 Tele Atlas © 2010 Europa Technologies US Dept of State Geographer

















#### Types of Plate Boundary



Thursday, January 6, 2011



#### Types of Plate Boundary



Thursday, January 6, 2011











http://earthquake.usgs.gov/earthquakes/world/seismicity/index.php



 Structure and Properties of Earth's Interior

- Structure and Properties of Earth's Interior
- Dynamics of Plate Tectonics/Global Mantle Convection

- Structure and Properties of Earth's Interior
- Dynamics of Plate Tectonics/Global Mantle Convection
- **Dynamics** of Plate Boundaries
  - Physics/Predictability of Earthquakes and Volcanoes

## What we actually know

- Detailed surface plate motions to ~200 Ma
- Geophysical Observations
  - Earthquake locations, Seismograms, Topography, Gravity, Magnetics
- Geochemical Observations
  - composition of earth materials (periodic table plus half the table of isotopes)

## What we actually know

- Detailed surface plate room to ~200 Ma
- Geophysical Observations
  - Earthquake locations, Seismograms, Topograph, Sravity, Magnetics
- Goothemizar Observations

composition of earth materials (periodic table plus half the table of isotopes)

 Quantitative Models provide the link between what we want to know and what we can actually observe.

- Quantitative Models provide the link between what we want to know and what we can actually observe.
- Advanced computation has always been an important component of solid earth geoscience because the Earth is
  - too big, too slow and can't build the laboratory experiment (similar to astrophysics)



### 2 of 6 2010 Gordon

#### **Bell finalists were in**

Filter

solid ëarth Geoscience

PRESENTATION	SPEAKER
190 TFlops Astrophysical N-body Simulation on a Cluster of GPUs	Tsuyoshi Hamada, Keigo Nitadori
Extreme-Scale AMR	Carsten Burstedde, Omar Ghattas, Michael Gurnis, Tobin Isaac, Georg Stadler, Tim Warburton, Lucas Wilcox
Scalable Earthquake Simulation on Petascale Supercomputers SC is the Internatio High Performance of Storage and Analys	Yifeng Cui, Kim B. Olsen, Thomas H. Jordan, Kwangyoon L SEARCH Zhou, Patrick Struan, Daniel Roten, Geoffrey Ely, Dhabaleswar K. Panda, Amit Chourasia, John Levesque, Steven M. Day, Philip Maechling
Multiscale Simulation of Cardiovascular flows on the IBM Bluegene/P: Full Heart-Circulation System at Red-Blood Cell Resolution	Amanda Peters, Simone Melchionna, Massimo Bernaschi, Sauro Succi, Efthimios Kaxiras, Mauro Bisson, Jonas Latt, Jov Sırcar
Petascale Direct Numerical Simulation of Blood Flow on 200K Cores and Heterogeneous Architectures	Abtin Rahimian, Ilya Lashuk, Shravan Veerapaneni, Aparna Chandramowlishwaran, Dhairya Malhotra, Logan Moon, Rahul Sampath, Aashay Shringarpure, Jeffrov Vettor, Richard Vuduc, Derns Zorin, George Biros
Toward First Principles Electronic Structure Simulations of Excited	Anton Kozhevnikov, Adol a liluz, Thomas C. Schulthess



### 2 of 6 2010 Gordon

#### **Bell finalists were in**

Filter

solid ëarth Geoscience

PRESENTATION	SPEAKER
190 TFlops Astrophysical N-body Simulation on a Cluster of GPUs	Tsuyoshi Hamada, Keigo Nitadori
Extreme-Scale AMR	Carsten Burstedde, Omar Ghattas, Michael Gurnis, Tobin Isaac, Georg Stadler, Tim Warburton, Lucas Wilcox
Scalable Earthquake Simulation on Petascale Supercomputers SC is the Internatio High Performance of Storage and Analys	Yifeng Cui, Kim B. Olsen, Thomas H. Jordan, Kwangyoon L SEARCH Zhou, Patrick Sman, Daniel Roten, Geoffrey Ely, Dhabaleswar K. Panda, Amit Chourasia, John Levesque, Steven M. Day, Philip Maechling
Multiscale Simulation of Cardiovascular flows on the IBM Bluegene/P: Full Heart-Circulation System at Red-Blood Cell Resolution	Amanda Peters, Simone Melchionna, Massimo Bernaschi, Sauro Succi, Efthimios Kaxiras, Mauro Bisson, Jonas Latt, Jov Sırcar
Petascale Direct Numerical Simulation of Blood Flow on 200K Cores and Heterogeneous Architectures	Abtin Rahimian, Ilya Lashuk, Shravan Veerapaneni, Aparna Chandramowlishwaran, Dhairya Malhotra, Logan Moon, Rahul Sampath, Aashay Shringarpure, Jeffrov, Vetter, Richard Vuduc, Vetter, Richard Vuduc, Vetter, Sorin, George Biros
Toward First Principles Electronic Structure Simulations of Excited	Anton Kozhevnikov, Adolen



### 2 of 6 2010 Gordon

#### **Bell finalists were in**

Filter

solid ëarth Geoscience

PRESENTATION	SPEAKER
190 TFlops Astrophysical N-body Simulation on a Cluster of GPUs	Tsuyoshi Hamada, Keigo Nitadori
Extreme-Scale AMR	Carsten Burstedde, Omar Ghattas, Michael Gurnis, Tobin Isaac, Georg Stadler, Tim Warburton, Lucas Wilcox
Scalable Earthquake Simulation on Petascale Supercomputers SC is the Internation High Performance Storage and Analys	Yifeng Cui, Kim B. Olsen, Thomas H. Jordan, Kwangyoon L SEARCH Zhou, Patrick Struan, Daniel Roten, Geoffrey Ely, Dhabaleswar K. Panda, Amit Chourasia, John Levesque, Steven
	M. Day, Philip Maechling
Multiscale Simulation of Cardiovascular flows on the IBM Bluegene/P: Full Heart-Circulation System at Red-Blood Cell Resolution	M. Day, Philip Maechling Amanda Peters, Simone Melchionna, Massimo Bernaschi, Sauro Succi, Efthimios Kaxiras, Mauro Bisson, Jonas Latt, Jov Sircar
Multiscale Simulation of Cardiovascular flows on the IBM Bluegene/P: Full Heart-Circulation System at Red-BloodCell ResolutionPetascale Direct Numerical Simulation of Blood Flow on 200K Cores and Heterogeneous Architectures	M. Day, Philip Maechling Amanda Peters, Simone Melchionna, Massimo Bernaschi, Sauro Succi, Efthimios Kaxiras, Mauro Bisson, Jonas Latt, Jov Sircar Abtin Rahimian, Ilya Lashuk, Shravan Veerapaneni, Aparna Chandramowlishwaran, Dhairya Malhotra, Logan Moon, Rahul Sampath, Aashay Shringarpure, Jeffron, Yetter, Richard Vuduc, Denis Zorin, George Biros

#### The Role of Computational Science in Solid





Carsten Burstedde,

Gurnis, Tobin Isaac, Georg Stadler, Tim

Omar Ghattas, Michael



log10(viscosity) (Pa s) 18.0 19.0 20.0 21.0 22.0 23.0 24.0



3-D FEM AMR Mantle
Convection code
150 million Elements
55,100 Cores (Jaguar)



**Extreme-Scale AMR** 

#### Scalable Earthquake Simulation on Petascale Supercomputers

Yifeng Cui, Kim B. Olsen, Thomas H. Jordan, Kwangyoon Lee, Jun Zhou, Patrick Small, Daniel Roten, Geoffrey Ely, Dhabaleswar K. Panda, Amit Chourasia, John Levesque, Steven M. Day, Philip Maechling

Domain: 810 x 405 x 100 km h\_min: 40 m # Dofs: 435 Billion # cores: 223,074 (Jaguar) 220 PFlops sustained for 24 hr highest frequency 2 hz



#### Scalable Earthquake Simulation on Petascale Supercomputers

Yifeng Cui, Kim B. Olsen, Thomas H. Jordan, Kwangyoon Lee, Jun Zhou, Patrick Small, Daniel Roten, Geoffrey Ely, Dhabaleswar K. Panda, Amit Chourasia, John Levesque, Steven M. Day, Philip Maechling

Domain: 810 x 405 x 100 km h\_min: 40 m # Dofs: 435 Billion # cores: 223,074 (Jaguar) 220 PFlops sustained for 24 hr highest frequency 2 hz



- 3 Principal Problems in Computational Geodynamics
  - Computational Seismology
  - Solid Mechanics: Mantle Convection, Continental Deformation, Earthquake Physics
  - Coupled Fluid/Solid Mechanics: Magma dynamics, subsurface flow/oil,water,gas

### The Challenge

- Putting it all together:
  - Develop Flexible, Interoperable, Open Source, high performance computational tools for exploring a wide range of multiscale/multi-physics geodynamic models.
  - Use any insight gained to understand both fundamental Earth Science and guide policy/ mitigate against natural hazards.
- This is the goal of the Computational Infrastructure for Geodynamics (CIG) (www.geodynamics.org)

### **Computational Seismology**



Simulation of 2011 January 2, Mw =7.1 Chile Earthquake wavefield using SPECFem3D\_Globe. Red: upward motion Blue: downward motion. <u>http://global.shakemovie.princeton.edu</u>/ Tromp et al, 2010, *GJI* 183, 381-389

### Computational Seismology Data



Thursday, January 6, 2011

### Computational Seismology Sensors



Figure 1. Map showing locations of 1838 seismographic stations supported by members of the FDSN (yellow dots). At each of these locations, the near real-time system provides three-component normal-mode synthetics for the 1-D PREM (Dziewoński & Anderson 1981) and SEM synthetics for 3-D model S362ANI (Kustowski *et al.* 2008) plus Crust2.0 (Bassin *et al.* 2000). The synthetics capture R1 and G1 at all epicentral distances for CMT events with  $M_{\rm W} < 7.5$ , and R2 and G2 for CMT events with  $M_{\rm W} \ge 7.5$ .
Computational Seismology Fundamental Questions Given heterogeneous distribution of sources (plate boundaries) and sparse set of receivers, can we

- Accurately locate Earthquakes?
- Infer dynamics of earthquake rupture? (Eq. Seismology)
- Develop high resolution image of earth's interior? (Structural Seismology)
- To do all of this requires modeling and extracting information from seismograms

# Computational Seismology The Forward Problem

Strong Form: Elastic Wave propagation

$$\rho \mathbf{u}_{tt} = \mathbf{\nabla} \cdot \boldsymbol{\sigma} + \mathbf{f}$$

$$\boldsymbol{\sigma} \cdot \mathbf{n} = \mathbf{0} \quad \text{on} \quad \partial \Omega$$

$$\mathbf{u} = \mathbf{0}, \quad \mathbf{u}_t = \mathbf{0} \quad \text{at} \quad \mathbf{t} = 0$$

#### where

elastic displacement field:

stress tensor:

strainrate tensor:

Earthquake Moment tensor Source:  $\mathbf{f} = -\mathbf{M}\delta(\mathbf{x} - \mathbf{x}_s)$ 

 $\begin{aligned} \mathbf{u}(\mathbf{x}, t) \\ \boldsymbol{\sigma} &= \mathbf{C} : \varepsilon \\ \varepsilon &= 1/2(\boldsymbol{\nabla}\mathbf{u} + \boldsymbol{\nabla}\mathbf{u}^{T}) \\ \mathbf{f} &= -\mathbf{M}\delta(\mathbf{x} - \mathbf{x}_{s}) \end{aligned}$ 

#### For isotropic Elastic media

$$\rho \mathbf{u}_{tt} = \boldsymbol{\nabla} \cdot \boldsymbol{\mu} (\boldsymbol{\nabla} \mathbf{u} + \boldsymbol{\nabla} \mathbf{u}^{T}) + \boldsymbol{\nabla} (k - 2\boldsymbol{\mu}/3) \boldsymbol{\nabla} \cdot \mathbf{u} + \mathbf{f}$$

# Computational Seismology The Forward Problem

#### Weak Form

Choose test-functions  $\mathbf{w}$  and trial functions  $\mathbf{u} \in \mathcal{V}$  s.t.

$$\int_{\Omega} \rho \mathbf{w} \cdot \mathbf{u}_{tt} d\mathbf{V} = \int_{\Omega} \nabla \mathbf{w} : \sigma d\mathbf{V} + \mathbf{M} : \nabla \mathbf{w}(\mathbf{x}_s) \mathbf{S}(t)$$

$$\mathbf{u} = \mathbf{0}, \quad \mathbf{u}_t = \mathbf{0} \quad \text{at} \quad \mathbf{t} = 0$$

- Note: Free stress Boundary conditions σ · n = 0 are automatically included as natural boundary conditions.
- Issue is simply choice of discrete function space  $\mathcal{V}$  for test functions **w** and **u**.
- Once chosen, the problem assembles into simple discrete wave equation

$$M\ddot{\mathbf{d}} + K\mathbf{d} = \mathbf{f}$$

for displacements **d**.

Thursday, January 6, 2011

# Computational Seismology Spectral Element methods



# Computational Seismology Spectral Element methods



A few nice Computational Features

Diagonal Mass Matrix: Lagrange Polynomials are "orthogonal" under GLL quadrature rules
Assembly parallelizes/vectorizes very well

4, 3-D hexahedral reference elements showing 5^3 dofs/element (4th order)

# Computational Seismology Spectral Element methods





#### Global Hexahedral mesh "cubed sphere"

Vertical structure showing crustal model and doubling layers

### Computational Seismology The Forward Problem

Discrete Form

$$M\ddot{\mathbf{d}} + K\mathbf{d} = \mathbf{f}$$

where M is a diagonal mass matrix, K(C) is the stiffness matrix, d is discrete vector of displacements.

#### Explicit Time Marching Scheme (Newmark)

Define Acceleration: 
$$\mathbf{a}_k = \ddot{\mathbf{d}}_k = M^{-1}[-K\mathbf{d}_k + \mathbf{f}_k]$$
  
Define Velocity:  $\mathbf{v}_k = \dot{\mathbf{d}}_k$   
Initialize :  $\mathbf{d}_0 = \mathbf{v}_0 = \mathbf{0}$ ,  $\mathbf{a}_0 = M^{-1}\mathbf{f}_0$   
for  $n = 1, 2, \dots$  do {loop until  $t = T$ }  
 $\mathbf{d}_n = \mathbf{d}_{n-1} + \Delta t \mathbf{v}_{n-1} + \frac{\Delta t^2}{2} \mathbf{a}_{n-1}$   
 $\mathbf{v}_n = \mathbf{v}_{n-1} + \frac{\Delta t}{2} [\mathbf{a}_{n-1} + \mathbf{a}_n]$   
end for

• CFL Stability Criteria: 
$$\Delta t \leq \alpha (\Delta x/c_p)_{min}$$
. ( $\alpha \sim 0.5$ )

Thursday, January 6, 2011

# **Computational Seismology** Full wavefield propagation

Scientific Mode Enabled :: Earthquake movies, 1D and 3D synthetic seismograms for seismologists.



SANTA CRUZ ISLANDS

# Computational Seismology Full wavefield propagation

7.1 Mw Jan 02, 2011 Chile Earthquake



# Computational Seismology Synthetic Seismograms



Figure 7. Vertical component record section comparing data (black) and SEM synthetics (red) for the 2008 September 3,  $M_w = 6.3$  Santiago del Estero, Argentina earthquake, which occurred at a depth of 571 km. The records are aligned on the *P* wave, plotted as a function of epicentral distance, and bandpass filtered between 17 and 60 s. Major seismological body wave arrivals are labelled. Epicentral distance is plotted to the left of each set of traces, and FDSN station identification codes are plotted to the right.

# Computational Seismology Synthetic Seismograms

7.1 Mw Jan 02, 2011 Chile Earthquake



### Computational Seismology Computational Cost/Performance

#### **Basic Scaling**

- Resolution depends on highest frequency wave we want to propagate accurately.
- Let  $\tau = 2\pi/\omega$  be the period of a wave with frequency  $\omega$
- Wavelength  $\lambda = \tau c$  depends on period and wavespeed
- Resolution  $h \propto \lambda \propto au_{min}$
- Time step limited by cfl condition  $\Delta t \propto h \propto au_{min}$
- Number of elements  $N_{el} \propto V/h^3 \propto \omega^3$
- Number of time steps  $N_t = T/\Delta t \propto \omega$
- Total ops  $O(\omega^4)$

### Computational Seismology Computational Cost/Performance

Routine Global Long period simulation (17 s)
 ~400 CPU cores in ~ 4 hours

2003 Gordon Bell Prize (Komatisch et. al, 2003)
 5 s minimum period (h~2.9 km)
 I 4.6 Billion dofs
 I 944 Vector processors on Earth Simulator
 30% peak on 38% of the machine 5Tflop sustained

 M8 (SCEC simulation 2010 GB Finalist)
 2 hz maximum frequency (1/2 s period) regional mesh with 435 Billion dofs
 223K opteron cores of Jaguar
 220 Pflops

# Computational Seismology The Inverse Problem



The Forward Problem: Given an earth model calculate synthetic seismograms at n locations.

The Inverse Problem: given mismatch between data and synthetic seismograms, refine the Earth model to minimize the misfit.

The Inverse Problem can be cast as a "PDE Constrained Optimization" problem solvable by adjoint methods

#### Computational Seismology PDE Constrained Optimization (the short course)

PDE Constrained Optimization: the generic problem

minimize  $J[u] = \frac{1}{2} \int_{\Omega} (u - d)^2 dV$ subject to  $\mathcal{L}(p)u = f$ , + BC's and IC's (PDE constraint)

#### with

- *u*: solution field
- d: data
- $\mathcal{L}(p)$ : Linear operator with parameters p

#### Define Lagrangian

$$L[\lambda, u, p] = \frac{1}{2} \int_{\Omega} (u - d)^2 dV + \int_{\Omega} \lambda \left[ \mathcal{L}(p)u - f \right] dV$$

- $\lambda(x, t)$  is a Lagrange multiplier
- Lagrangian provides weighted misfit between solution, data and PDE constraint.

#### Optimality conditions

Calculate the first variation and set to zero

$$\delta L = \delta L_{\lambda} + \delta L_{u} + \delta L_{p} = 0$$

where

$$\delta L_{\lambda} = \int_{\Omega} \left[ \mathcal{L}(p)u - f \right] \delta \lambda dV = 0$$
  
$$\delta L_{u} = \int_{\Omega} \left[ \left( u - d \right) + \mathcal{L}^{\dagger}(p)\lambda \right] \delta u dV = 0$$
  
$$\delta L_{p} = \int_{\Omega} \left[ \lambda G(p)u \right] \delta p dV = 0$$

*L*<sup>†</sup> is the adjoint operator defined by ∫<sub>Ω</sub> λLudV = ∫<sub>Ω</sub> uL<sup>†</sup>λdV

 Note: linear elastic wave propagation is *self-adjoint* s.t.
 *L*<sup>†</sup> = L

Thursday, January 6, 2011

#### Implications

- $\delta L_{\lambda} = 0$  implies that *u* satisfies the original PDE with forcing *f*
- $\delta L_u = 0$  implies that the Lagrange multiplier satisfies the adjoint PDE

$$\mathcal{L}^{\dagger}(p)\lambda = -(u-d)$$

with forcing driven by the mismatch between data and synthetics

 if u and λ satisfy their respective PDE's, then the gradient δL reduces to just model sensitivity which can be written in terms of a *sensitivity Kernel*

$$\delta L = \int K(u,\lambda,p) \delta p dV$$

where

$$K(u,\lambda,p)=\lambda G(p)u$$

Example: Waveform Tomography

• Given model p (e.g.  $\rho$ , C or  $v_p$ ,  $v_s$ ), solve the forward problem

$$\int_{\Omega} \rho \mathbf{w} \cdot \mathbf{u}_{tt} d\mathbf{V} = \int_{\Omega} \nabla \mathbf{w} : \sigma(\mathbf{u}) + \mathbf{M} : \nabla \mathbf{w}(\mathbf{x}_s) \mathbf{S}(t)$$

with  $\mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_t(\mathbf{x}, 0) = \mathbf{0}$ 

Solve the adjoint problem in reverse time (using the same code)

$$\int_{\Omega} \rho \mathbf{w} \cdot \hat{\mathbf{u}}_{tt} dV = \int_{\Omega} \nabla \mathbf{w} : \sigma(\hat{\mathbf{u}}) + \sum_{r} \int_{0}^{T} (u_{r} - d_{r}) dt$$

with  $\lambda(\mathbf{x}, t) = \hat{\mathbf{u}}(\mathbf{x}, T - t)$  and "IC's"  $\hat{\mathbf{u}}(\mathbf{x}, 0) = \hat{\mathbf{u}}_t(\mathbf{x}, 0) = \mathbf{0}$ 

• Calculate Sensitivity Kernels and optimize to minimize  $\delta L$  (e.g. CG, Newton, etc).

### Computational Seismology Example Sensitivity Kernel



Figure 10: (a) Vertical component synthetic velocity seismograms recorded at an epicentral distance of 60 for simulations accurate down to periods of 27 s (green), 18 s (red) and 9 s (blue), respectively. (b) Source-receiver cross-section of the  $K_{\alpha}$  kernel, defined by (4.27), for a 27 s P wave recorded at a station at an epicentral distance of 60°. The source and receiver locations are denoted with two small white circles. The unit of the sensitivity kernels is  $10^7 \text{ s/km}^3$  throughout this paper. (c)  $K_{\alpha}$  kernel for an 18 s P wave recorded at a station at an epicentral distance of  $60^{\circ}$ . (d)  $K_{\alpha}$  kernel for a 9 s P wave recorded at a station at an epicentral distance of  $60^{\circ}$ . (d)  $K_{\alpha}$  kernel for a 9 s P wave recorded at a station at an epicentral distance of  $60^{\circ}$ .

#### **Computational Seismology** Example 3-D Regional Waveform Tomography

#### **Geophysical Journal International**



Geophys. J. Int. (2010) 180, 433-462

doi: 10.1111/j.1365-246X.2009.04429.x

#### Seismic tomography of the southern California crust based on spectral-element and adjoint methods

#### Carl Tape,<sup>1\*</sup> Qinya Liu,<sup>2</sup> Alessia Maggi<sup>3</sup> and Jeroen Tromp<sup>4</sup>

<sup>1</sup>Seismological Laboratory, California Institute of Technology, Pasadena, CA 91125, USA. E-mail: carltape@gps.caltech.edu <sup>2</sup>Department of Physics, University of Toronto, ON, Canada

<sup>3</sup>Institut de Physique du Globe, Université de Strasbourg, Strasbourg, France

<sup>4</sup>Department of Geosciences and Program in Applied & Computational Mathematics, Princeton University, Princeton, NJ, USA

#### Full problem: 16 Iterations 6800 wavefield simulations 800,000 total cpu hours (178 cores)

#### **Computational Seismology** Example 3-D Regional Waveform Tomography

Seismic tomography of the southern California crust



#### Regional Models are critical for Earthquake hazard assessment (shaking)



I43 Earthquakes (beach balls)

•203 stations (triangles) used in inversion

• 91 Additional earthquakes used for validation.



Thursday, January 6, 2011

#### **Computational Seismology** Example 3-D Regional Waveform Tomography



Figure 5. The influence of sedimentary basins on the seismic wavefield. (a) Cross-section of the final  $V_S$  crustal model  $\mathbf{m}_{16}$ , containing the path from event 14179736 ( $\star$ ;  $M_w$  5.0, depth 4.9 km), beneath the Salton trough, to station LAF.CI ( $\nabla$ ; distance 263.5 km), within the Los Angeles basin. (b, left column) Data (black) and 1-D synthetics (red). (b, right column) Data (black) and 3-D synthetics for model  $\mathbf{m}_{16}$  (red). The seismograms are bandpass filtered over the period range 6–30 s. Z, vertical component, R, radial component, T, transverse component.

#### Influence of local structure (sedimentary basins) on shaking

# Computational Seismology Available Software

Source (F90): at CIG (<u>www.geodynamics.org</u>)





3-D Regional model v2.0.0 "Sesame" accepts arbitrary hexahedral meshes, Well interfaced with CUBIT (Sandia). Forward and Adjoint models, absorbing boundaries Open Source: GPL license

- Pre-Computed Synthetics:
  - 3-D Global: <u>http:/global.shakemovie.princeton.edu/</u>
  - Regional SC: <u>http://shakemovie.caltech.edu/</u>

# **Computational Seismology**



- Pre-Computed Synthetics:
  - 3-D Global: <u>http:/global.shakemovie.princeton.edu</u>/
  - Regional SC: <u>http://shakemovie.caltech.edu/</u>

### Computational Seismology GPU implementations

#### Dmitri Komatisch (U. Pau):

**Dimitri Komatitsch**, Fluid-solid coupling on a cluster of GPU graphics cards for seismic wave propagation, *Comptes Rendus de l'Académie des Sciences* – *Mécanique*, doi: 10.1016/j.crme.2010.11.007, in press (2011). <u>PDF reprint BibTeX</u>

**Dimitri Komatitsch**, Gordon Erlebacher, Dominik Göddeke and David Michéa, High-order finite-element seismic wave propagation modeling with MPI on a large GPU cluster, *Journal of Computational Physics*, vol. 229(20), p. 7692-7714, doi: 10.1016/j.jcp.2010.06.024 (2010). <u>PDF reprint BibTeX</u>

David Michéa and **Dimitri Komatitsch**, Accelerating a 3D finite-difference wave propagation code using GPU graphics cards, *Geophysical Journal International*, vol. 182(1), p. 389-402, doi: 10.1111/j.1365-246X.2010.04616.x (2010). <u>PDF reprint BibTeX</u>

#### June 2010: a multi-GPU port of SPECFEM3D wins the BULL Joseph Fourier supercomputing award:





Prix Bull - Joseph Fourier en association avec GENCI

Pour le développement de la simulation numérique

### Computational Seismology GPU Cluster Configuration

D. Komatitsch et al./Journal of Computational Physics 229 (2010) 7692-7714



Fig. 9. Description of the cluster of 48 Teslas S1070 used in this study. Each Tesla S1070 has four GT200 GPUs and two PCI Express-2 buses (i.e., two GPUs share a PCI Express-2 bus). The GT200 cards have 4 GB of memory, and the memory bandwidth is 102 GB/s with a memory bus width of 512 bit. The Teslas are connected to BULL Novascale R422 E1 nodes with two quad-core Intel Xeon X5570 Nehalem processors operating at 2.93 GHz. Each node has 24 GB of RAM. The network is a non-blocking, symmetric, full duplex Voltaire InfiniBand double data rate (DDR) organized as a fat tree.

#### •48 Nodes: each with

- | SI070 (4 GT200 GPUs)
- •2 quad-core 2.93GHz Nehalems
- Infiniband connect between nodes
- •Total: 192 GPUs + 384 CPU cores

7706

# CPU vs. GPU Performance

**Dimitri Komatitsch**, Gordon Erlebacher, Dominik Göddeke and David Michéa, High-order finite-element seismic wave propagation modeling with MPI on a large GPU cluster, *Journal of Computational Physics*, vol. 229(20), p. 7692-7714, doi: 10.1016/j.jcp.2010.06.024 (2010). <u>PDF reprint BibTeX</u>



#### Weak Scaling Results

- Computational Seismology is a beautiful computational problem
  - Well Posed Forward problem
  - Explicit, single physics & Linear
  - Highly Parallel (Multicore, Vector and GPU)

- Computational Seismology is a beautiful computational problem
  - Well Posed Forward problem
  - Explicit, single physics & Linear
  - Highly Parallel (Multicore, Vector and GPU)
- Output is directly comparable to Data! (seismograms)

- Computational Seismology is a beautiful computational problem
  - Well Posed Forward problem
  - Explicit, single physics & Linear
  - Highly Parallel (Multicore, Vector and GPU)
- Output is directly comparable to Data! (seismograms)
- Inverse problem expensive, but tractable
  - Self-Adjoint linear problem = code reuse
  - Complexity is maneagable and I0x GPU speedup will translate directly to inverse problem

- Computational Seismology is a beautiful computational problem
  - Well Posed Forward problem
  - Explicit, single physics & Linear
  - Highly Parallel (Multicore, Vector and GPU)
- Output is directly comparable to Data! (seismograms)
- Inverse problem expensive, but tractable
  - Self-Adjoint linear problem = code reuse
  - Complexity is maneagable and I0x GPU speedup will translate directly to inverse problem
- Near State of the art codes publically available through CIG (Open Source GPL)

### Computational Seismology Caveats
Don't get used to this ;^)

- Don't get used to this ;^)
- Computational Seismology is the most mature (and in some sense easiest) HPC problem in Solid Earth Geophysics

- Don't get used to this ;^)
- Computational Seismology is the most mature (and in some sense easiest) HPC problem in Solid Earth Geophysics
- Extremely important for imaging current Earth structure and estimating Seismic Hazard

- Don't get used to this ;^)
- Computational Seismology is the most mature (and in some sense easiest) HPC problem in Solid Earth Geophysics
- Extremely important for imaging current Earth structure and estimating Seismic Hazard
- But doesn't yield Earth Dynamics.

- Don't get used to this ;^)
- Computational Seismology is the most mature (and in some sense easiest) HPC problem in Solid Earth Geophysics
- Extremely important for imaging current Earth structure and estimating Seismic Hazard
- But doesn't yield Earth Dynamics.
  - That's a much harder problem (to be continued...)