## Prospects for Seismic Inversion on Petaflop Systems

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#### Prospects for Seismic Inversion on Petaflop Systems

#### Prospects

- Current situation: funding, expectations, challenges
- of Seismic Inversion
  - full waveform inversion in 3D
  - least-squares observation and modifications
  - inexact Newton-Krylov iterative algorithm
- on Petaflop Systems
  - large problems on large clusters of computers
  - a very specialized view on computation:

#### "Does it scale?"

#### "Does it scale?" – What is the meaning?

"Strong scaling" – often unrealistic

- Fix problem size (e.g. size of the domain, frequency):
- Runtime decrease in proportion to resource increase?
- "Weak scaling" widely accepted criterion
- Fix problem size per processor (e.g. space/time variables)
- Runtime stays constant while increasing #processors?

#### Some things that do not scale:

- Hard disk read/write (limited resource, slow bandwidth)
- Dense matrices (assembly, storage, matrix-vector product N^2)
- Matrix inversion (storage N^2, runtime N^3)
- Implicit PDE solvers (limited by network topology, bandwidth)
- Steepest descent minimization (#iterations depend on N)

Prospects for Seismic Inversion On Petaflop Systems → 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

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 billion x 4000 x 10 =  $10^{15}$   $\longrightarrow$  1 Petaflop

- 25 million grid boxes

Flop – "Floating Point Operation"

#### On the Road to Petascale Computation

#### Identification of possible scientific breakthroughs

- SCaLeS report, Petascale Collaboratory for Geosciences
- President's American Competitiveness Initiative (ACI)

#### Aggressive programs for petaflops performance

- NSF Track 1 Petascale Acquisition, DOE SC @ ORNL, ANL
- Cost for NSF and DOE/SC Petaflop systems alone: >\$1B
- First peak petaflop machine should appear in 2008

#### **Opportunities**

- Now it is up to the science & engineering communities to make effective use of these systems
- Many of the grand challenge problems facing society today are related to the geosciences
- High performance computing is "popular" but for how long?

Performance is Flop per Second: How expensive are sustained Flop/s?

#### Human

- 0.1 Flop/s \$100,000

#### Laptop

- 10 Gigaflop/s \$1,500
- Selfmade cluster
- 1 Teraflop/s \$200,000
- The world's biggest systems in 2011
- 1 Petaflop/s \$200,000,000 each

Does it scale (hardware/money)? – Probably. Does it scale (potential for waste/failure)? – Definitely.

#### Challenges of Petascale Computation

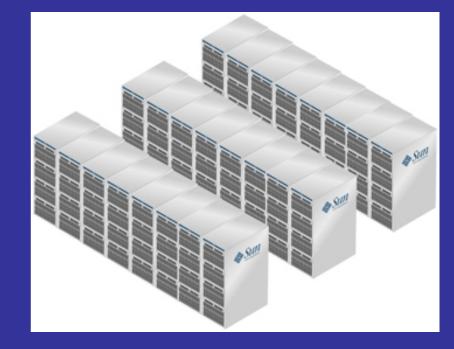
- Does it scale (unprecedented hardware complexity)? hopefully.
  - o 500K 1M cores
  - o Multicore processors, specialized accelerator chips
    - AMD: GP-GPU Intel: 80-core teraflop box
    - IBM: cell processor FPGAs
    - Cray: multithreading + multicore scalar
    - Multiple processors inside SMP box
    - Complex network topology
- Does it scale (numerical algorithms)?
   that's us <</li>
  - o Good news: in principle, PDE solvers should scale... but in practice?
    - anisotropies, heterogeneities, multiphysics, nonlinearities, ...
    - dynamic adaptivity, free boundary/interface problems, ...
  - o Growing algorithmic and programming complexity
    - Deep nesting of control flow / data structures

#### Building a petaflops machine is unquestionably hard. But using it is even harder!

#### New Sun/AMD system at Texas Advanced Computing Center, UT-Austin

- New \$59M NSF award to UT deploy and maintain Sun/AMD "Track 2" supercomputer
- Collaboration between TACC, ICES, Cornell, and Arizona St.
- Expected final configuration in November 2007:
  - o Deerhound-based (quad-core, 4-way)
  - o 530 Teraflop/s
  - o >62,000 cores
  - o 125 TB memory
  - o 1.9 PB disk





The billion dollar question: Can we scale up our simulations to capitalize on O(10<sup>5</sup>) CPUs?

#### Overall scalability requires:

- System scalability
- Implementation scalability
- Algorithmic scalability
  - Some of the most powerful and algorithmicallyscalable numerical algorithms and schemes also have the most complex data structures and implementation requirements
    - Multigrid, AMR, fast multipole, ...
  - o Focus of talk: how scalable is seismic inversion?
    - Part 1: scalability of forward solver
    - Part 2: scalability of inverse method

#### Earthquake wave propagation model

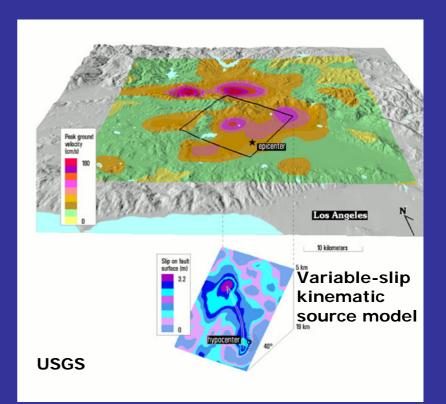
$$\nabla \cdot \left[ \mu \left( \nabla u + \nabla u^{\mathsf{T}} \right) + \lambda (\nabla \cdot u) I \right] = \rho \ddot{u} - b \text{ in } \Omega \times (0, T)$$
$$\left[ \mu \left( \nabla u + \nabla u^{\mathsf{T}} \right) + \lambda (\nabla \cdot u) I \right] n = L^{AB} u \text{ on } \partial \Omega \times (0, T)$$
$$u = 0 \text{ on } \Omega \times \{t = 0\}$$
$$\dot{u} = 0 \text{ on } \Omega \times \{t = 0\}$$

+Rayleigh attenuation model

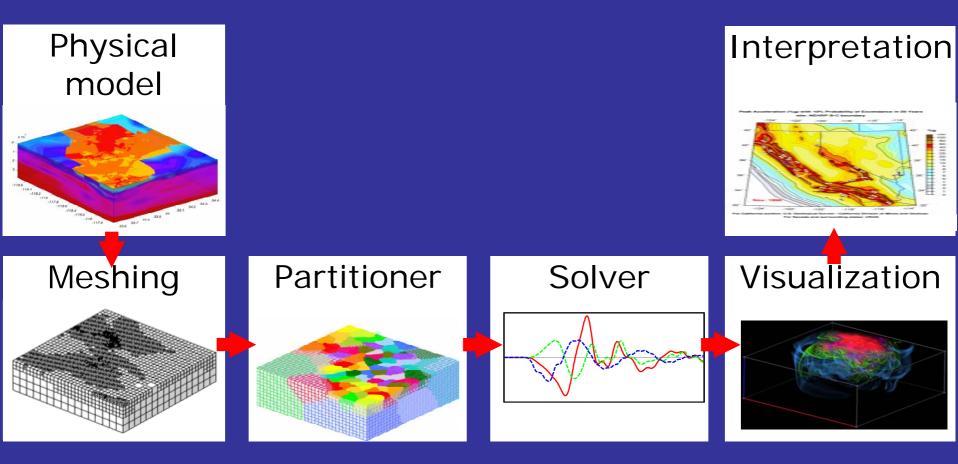
 $egin{aligned} u(x,t) &:= ext{displacement} \ &
ho &:= ext{material density} \ &\mu,\lambda &:= ext{elastic parameters} \ b(x,t) &:= ext{rupture force, e.g. for point source} \ &:= ext{-} \mu v A f(t) M oldsymbol{
abla} \delta(x-oldsymbol{\xi}) \end{aligned}$ 

 $L^{AB}$  is 0 on free surfaces, and is given by Stacy's absorbing boundary condition on truncated surfaces:

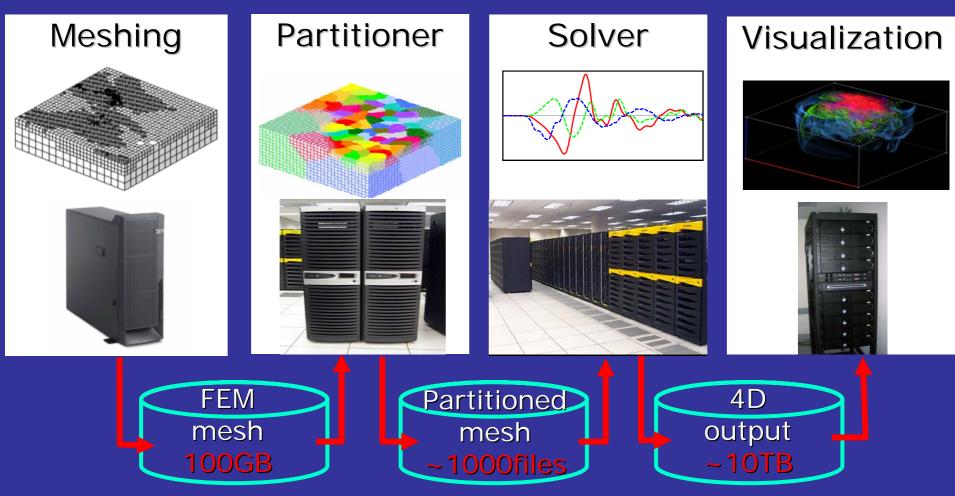
$$\begin{split} \boldsymbol{L}^{AB}\boldsymbol{u} &\equiv \begin{bmatrix} -d_1\frac{\partial}{\partial t} & c_1\frac{\partial}{\partial \tau_1} & c_1\frac{\partial}{\partial \tau_2} \\ -c_1\frac{\partial}{\partial \tau_1} & -d_2\frac{\partial}{\partial t} & 0 \\ -c_1\frac{\partial}{\partial \tau_2} & 0 & -d_2\frac{\partial}{\partial t} \end{bmatrix} \begin{cases} u_n \\ u_{\tau_1} \\ u_{\tau_2} \end{cases} \\ \boldsymbol{u}_{\tau_2} \end{cases} \\ \boldsymbol{c}_1 &= -2\mu + \sqrt{\mu(\lambda + 2\mu)}, \\ d_1 &= \sqrt{\rho(\lambda + 2\mu)}, \\ d_2 &= \sqrt{2\mu} \end{split}$$



# Forward modeling toolchain

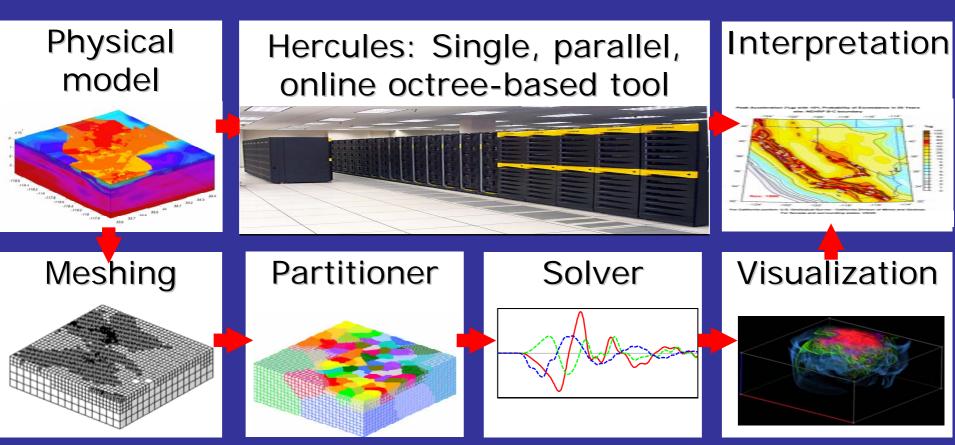


# Pitfalls of old system Different computing systems I/O and network bandwidth bound Complex data format conversions



## End-to-end parallelism (Tiankai Tu and Hongfeng Yu)

- Avoid large file I/O
- JPEG outputs
- Enable online steering



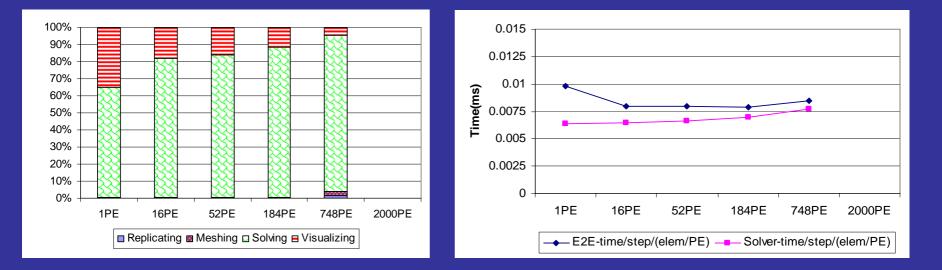
#### Isogranular Scalability (55 TF/s TACC Lonestar)

LA Basin (100km x 100km x 37.5 km), SCEC CVM Version 2.0; minimum shear wave velocity 100m/s

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Meshing:  $O(N \log E) = O(N \log N)$ Wave propagation solver:  $O(N T) = O(N^{4/3})$ Volume rendering:  $O(XY E^{1/3} \log E) = O(XY N^{1/3} \log N)$ N = # grid points; E = # elements; T = # time steps; (X, Y) = pixels in canvas

#### Performance data (AlphaServer at PSC)



#### Isogranular scalability:

• End-to-end: up to 534M grid pts, 81% efficiency from 1 to 784 processors

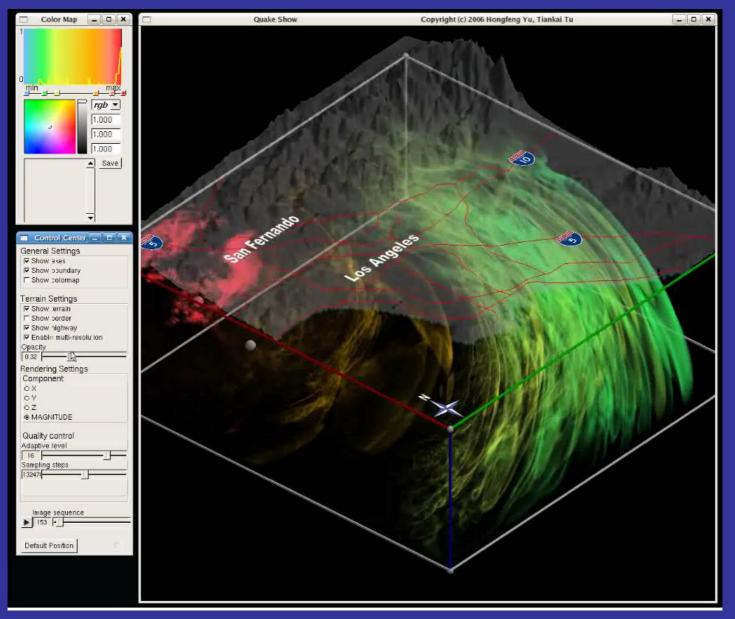
#### Fixed-size scalability:

- Meshing + solver: 134M grid pts, 84% efficiency on 2048 processors (base 128PEs)
- End-to-end: 134M grid pts, 76% efficiency on 748 processors (base 128PEs)

#### Processor utilization:

• ~655 MFlops/sec/PE; 33% of the peak performance (2GFlops/sec/PE).

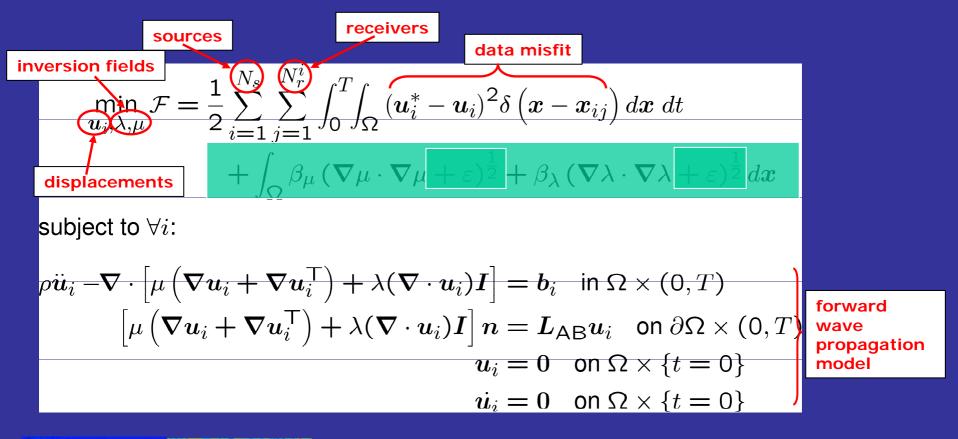
# Example: 1994 Northridge earthquake simulation (2006) (real-time on 2000 cores of TACC Dell/Woodcrest Lonestar)

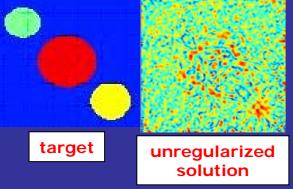


### Full waveform inversion: Challenges

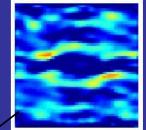
- Inverse problem can be highly nonlinear even when forward problem is linear
- Inverse operator is non-local, non-causal
- Need to build on large body of algorithms, libraries, and software for forward simulation
- Numerous forward simulations required for an inverse solution
- Numerous inverse solutions required to estimate best regularization parameter
- Want to estimate not just mean of parameters, but also variance (or better: distribution)
- Significant work by: Symes, Tarantola, Chavent, Mora, Jordan, Tromp, Pratt, etc.

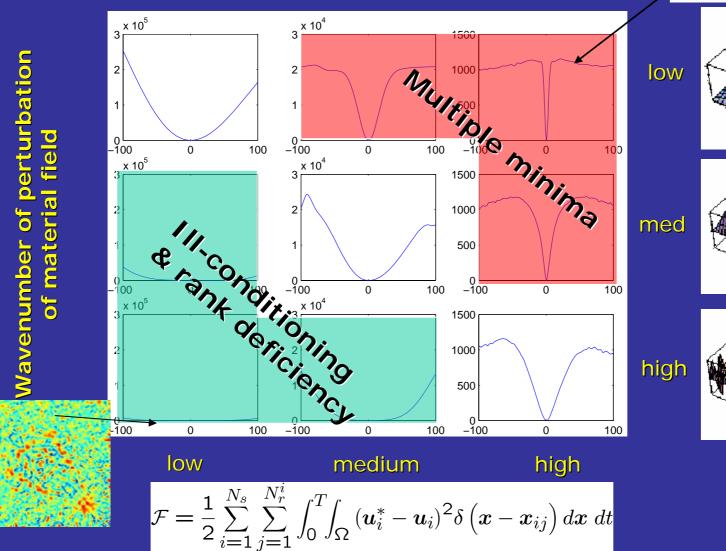
# Least squares parameter estimation formulation of inverse wave propagation



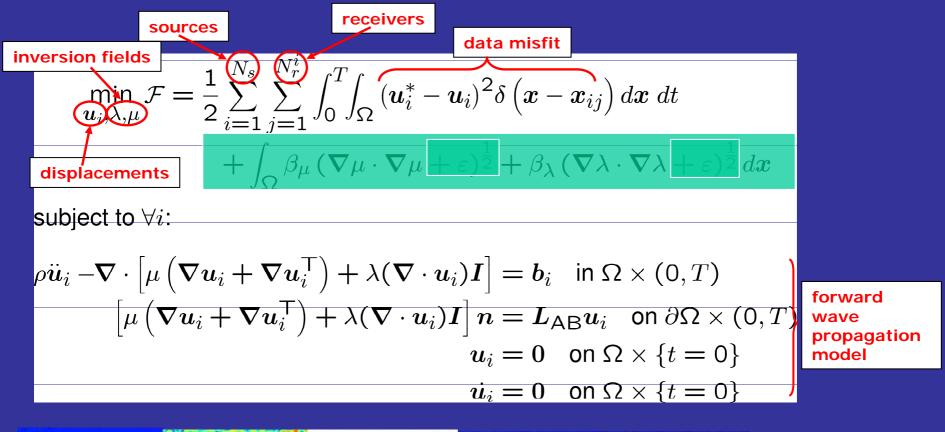


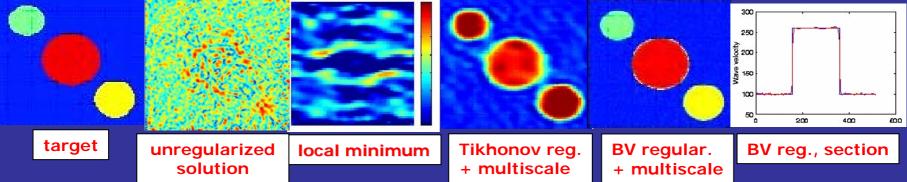
# Behavior of misfit function *F* in direction of material perturbation



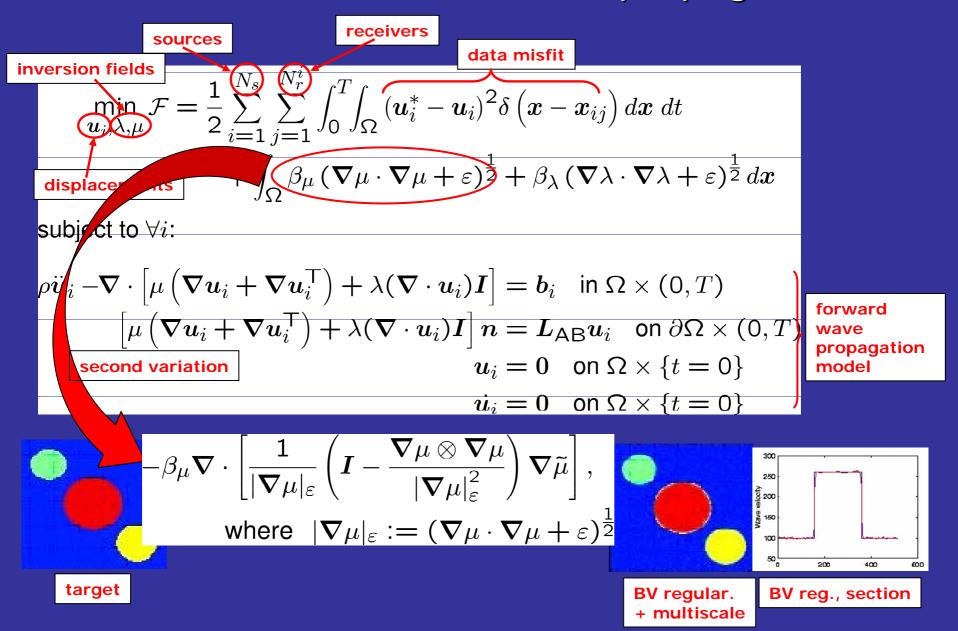


# Least squares parameter estimation formulation of inverse wave propagation





# Least squares parameter estimation formulation of inverse wave propagation



#### Lagrangian and weak form of optimality system

$$\begin{split} \mathcal{L}(u,p,\mu) &:= \frac{1}{2} \sum_{j=1}^{N_r} \int_0^T \int_{\Omega} (u-u^*)^2 \delta(x-x_j) \, dx \, dt \ + \ \beta \int_{\Omega} |\nabla \mu|_{\varepsilon} \, dx \\ &+ \int_0^T \int_{\Omega} (\mu \nabla u \cdot \nabla p - \rho u_t \, p_t) \, dx \, dt \ - \int_0^T \int_{\Sigma} \mu u_0 g \nabla p \cdot \boldsymbol{n}_{\Sigma} \, ds \, dt \ - \int_0^T \int_{\Gamma_{AB}} u_t p \sqrt{\rho \mu} \, ds \, dt \end{split}$$

×

### Strong form of first order necessary conditions



#### A Gauss-Newton-Schur-CG method

#### The Gauss-Newton step:

$$\begin{array}{c} \mathcal{B} & \mathcal{C}^{*}(p) & \mathcal{A}^{*}(\mu) \\ \hline \mathcal{C}(p) & \mathcal{R}(\mu) & \mathcal{D}^{*}(u) \\ \mathcal{A}(\mu) & \mathcal{D}(u) & 0 \end{array} \right] \left\{ \begin{array}{c} \tilde{u} \\ \tilde{\mu} \\ \tilde{p} \end{array} \right\} = - \left\{ \begin{array}{c} \mathcal{L}_{u}(u,\mu,p) \\ \mathcal{L}_{\mu}(u,\mu,p) \\ \mathcal{L}_{p}(u,\mu) \end{array} \right\}$$

A linear Schur complement method:

 $\left(\mathcal{D}^{*}\mathcal{A}^{*^{-1}}\mathcal{B}\mathcal{A}^{-1}\mathcal{D}-\mathcal{D}^{*}\mathcal{A}^{*^{-1}}\mathcal{C}-\mathcal{C}\mathcal{A}^{-1}\mathcal{D}+\mathcal{R}
ight) ilde{\mu}=\mathcal{D}^{*}\mathcal{A}^{*^{-1}}\mathcal{L}_{u}-\mathcal{L}_{\mu}$ 

- Hostead, soble & Straightfgate gradients approach intractates in gettor progests problem, versionate:
  - o ear Minen Eisenstato Walkerons to set up linear system
  - e gleenvithline search or trust region
  - e eachur Gotterationarequires hatenwardr bradjoint wave propagation -> parallelizes as well as forward
  - o problem (Nsforw/adj wave propagations for multiple for IH2 (Asrnodel, zettascale/yottascale computing sources) arrives in ~2050 per Demi Moore's law)
  - o construction of preconditioner difficult, since Hessian not formed explicitly

# Algorithmic scalability for 3D acoustic inversion example

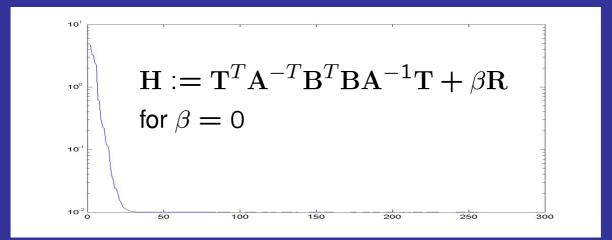
material grid	Picard-Gauss-Newton-Krylov iter, no PC			Picard-Gauss-	Newton-Krylov i	iter, LBFGS/2SR PC
	nonlinear iter	total linear iter	avg linear iter	nonlineariter	total lineariter	avg lineariter
$2^{3}$	6	31	5.2	6	13	2.2
33	11	121	11.0	11	39	3.5
$5^{3}$	18	321	17.8	17	144	8.5
9 <sup>3</sup>	13	614	47.2	12	249	21.0
$17^{3}$	11	1413	128.5	12	396	33.0
$33^{3}$	17	1445	85.0	25	439	17.6
$65^{3}$	19	1923	101.2	19	370	19.5
$129^{3}$	21	2003	95.4	22	436	19.8
		•				

Mesh independence of nonlinear iterations

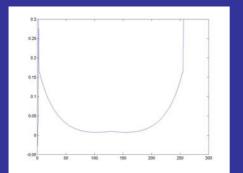
Mesh independence of linear iterations

But even with mesh independence, # of wave propagations still large!

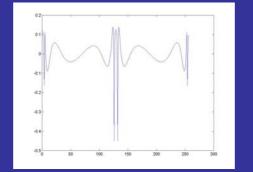
#### Motivation for reduced space CG solver



#### Spectrum of discrete reduced Hessian



Eigenvector for large eigenvalue



0.250.250.150.0550.0650.0650.0650.0650.075

Eigenvector for intermediate eigenvalue

Eigenvector for small eigenvalue

### Solution algorithm: Multilevel inexact Gauss-Newton-PCG

- Multilevel continuation over grid and source frequency
  - o Inexact Gauss-Newton nonlinear iteration
    - Conjugate gradient solution of reduced Hessian system (each matvec requires N<sub>s</sub> forward & adjoint wave propagation solutions)
      - Preconditioner:
        - » limited memory BFGS (Morales-Nocedal)
        - » initialized with several iterations of Frankel's method (two-step stationary method) to "invert" T + 0.00

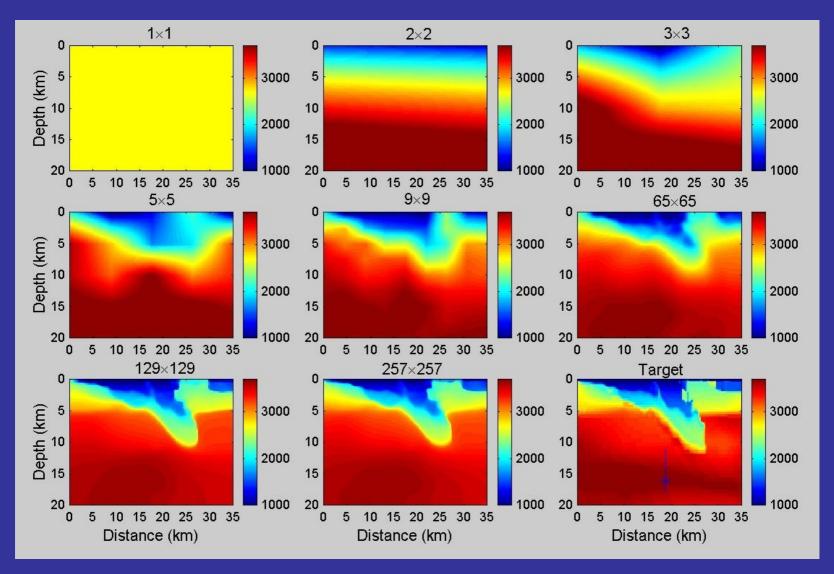
invert" 
$$\alpha \mathcal{I} + \beta \mathcal{F}$$

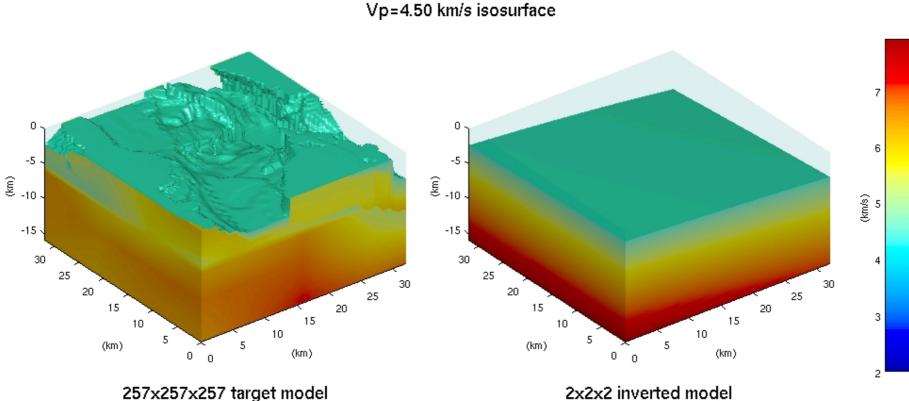
» Multigrid

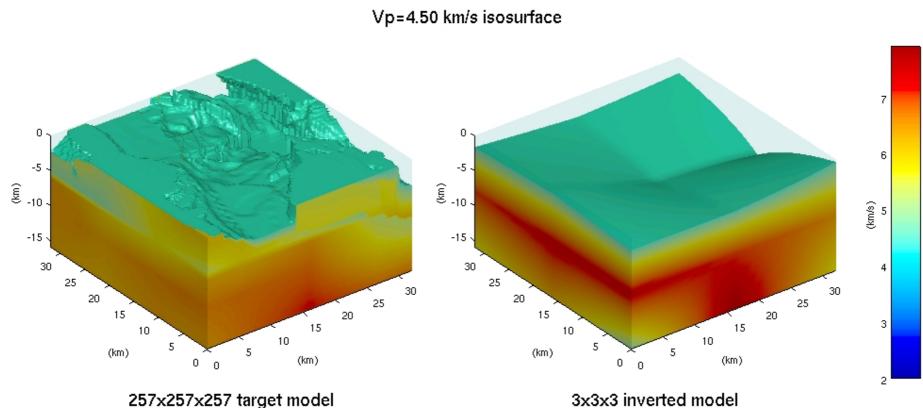
#### Inversion examples

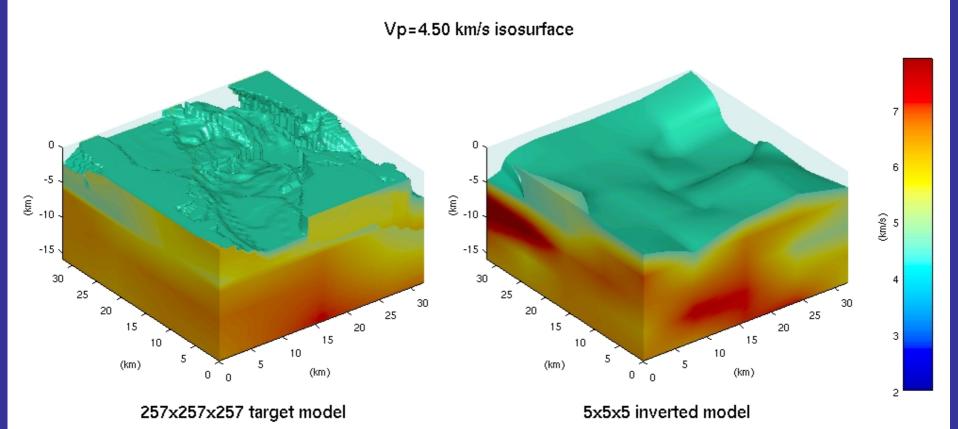
- 2D shear, 3D acoustic, and 3D elastic models
- Synthetic inversion (some with 5% added noise) using SCEC community velocity model
- Piecewise bi/trilinear finite element approximation of state, adjoint, and material property in space
- Explicit central difference time integration
- PETSc (<u>www.petsc.anl.gov</u>) implementation
- Up to 257x257x257 grid (17 million inversion parameters) on 2048 processors (~12h)
- Up to 225 surface receivers

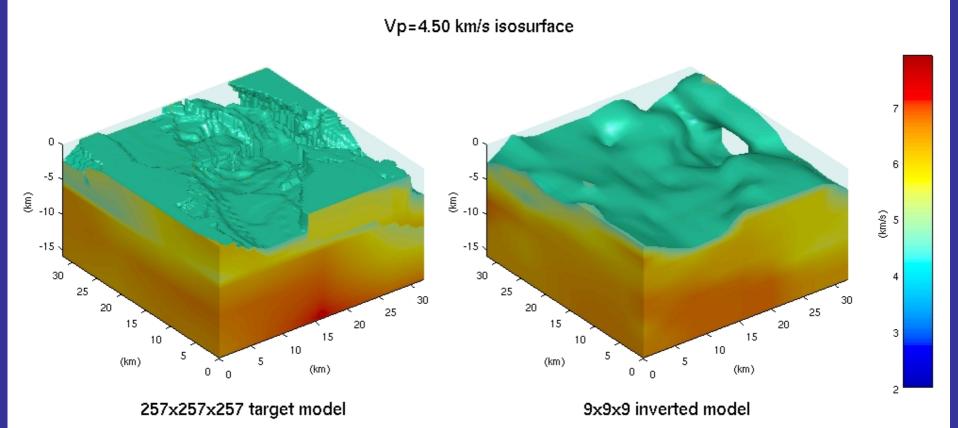
# Material inversion: multiscale continuation (64 receivers)

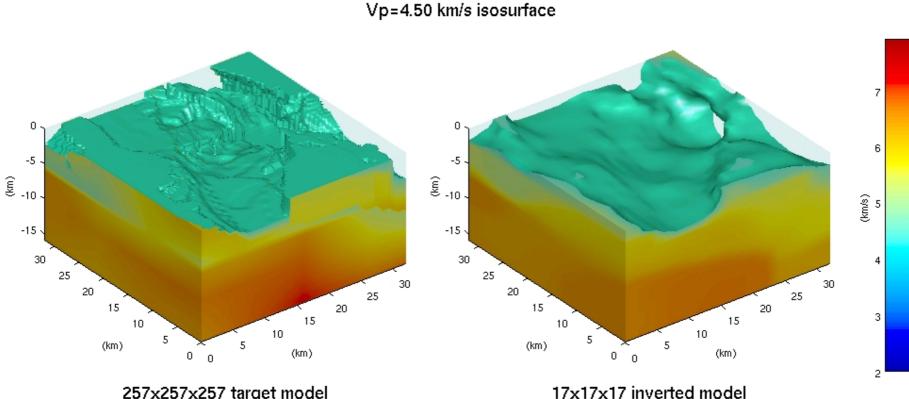




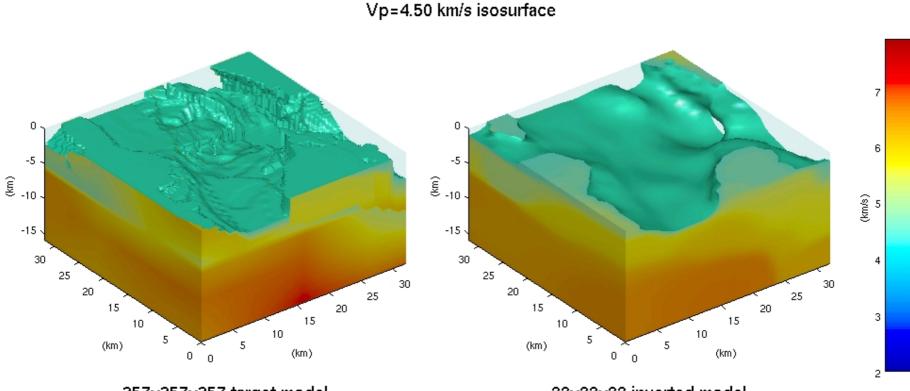






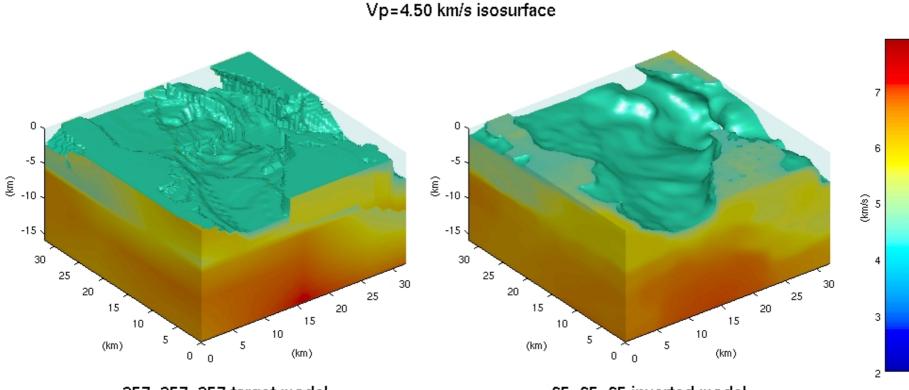


257x257x257 target model



33x33x33 inverted model

257x257x257 target model



65x65x65 inverted model

257x257x257 target model

Vp=4.50 km/s isosurface -5 -5 . 환 -10 <u>چ</u> ۱۰۰ (s/m/s) -15 --15 -(km) (km) (km) (km) 257x257x257 target model

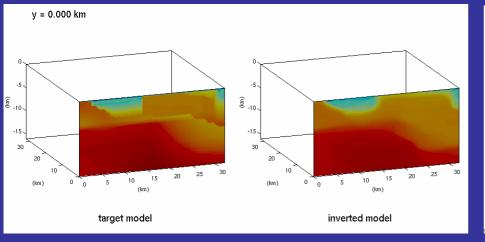
129x129x129 inverted model

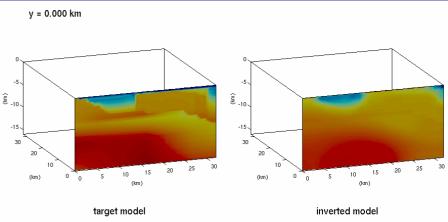
Vp=4.50 km/s isosurface -5 -5 َ اللَّٰ 10 ال <u>چ</u> ۱۰۰ (s/m/s) -15 --15 -(km) (km) (km) (km) 

257x257x257 inverted model

257x257x257 target model

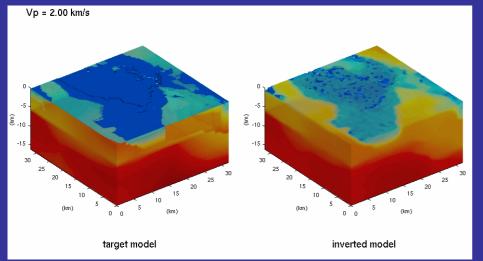
# Comparison of target and inverted material models: 3D acoustic and elastic





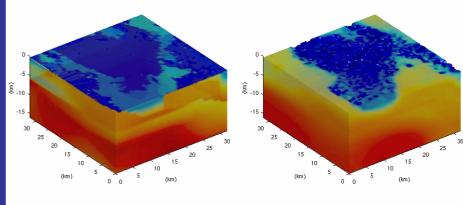
#### Acoustic medium, p-wave velocity

#### Elastic medium, s-wave velocity

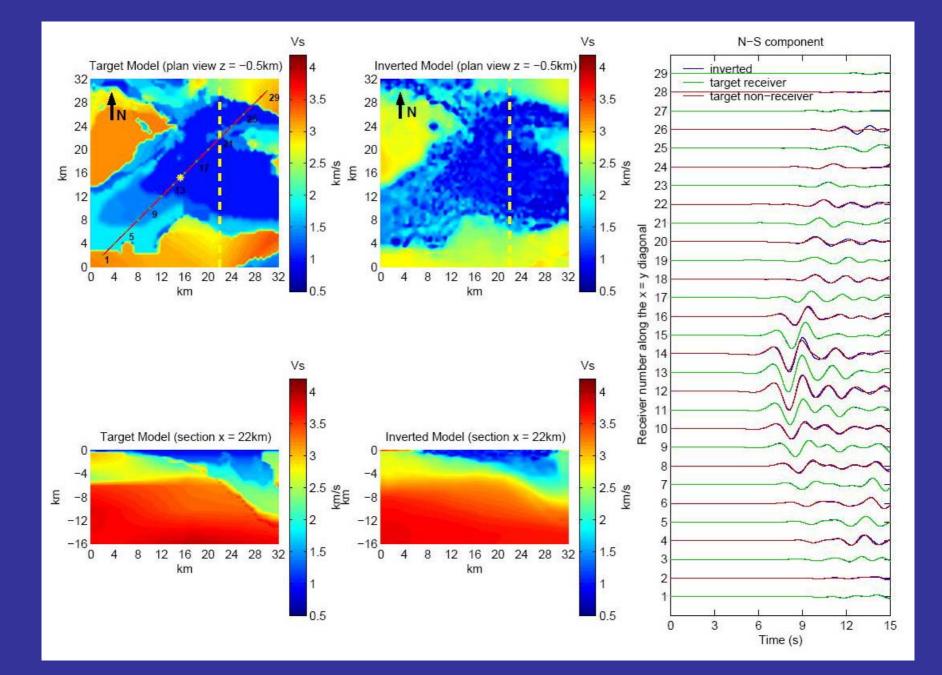


Vs = 1.00 km/s

target model



inverted model



# Prospects for 3D elastodynamic inversion with observations from multiple events?

- 4x2 earthquake simulations per CG iteration
- 20 CG iterations per Gauss-Newton iteration
- 20 Gauss-Newton iterations
- Inversion costs 4000x a single forward simulation
- Assume sustained petaflops machine has 100,000 8X faster CPUs (than Lonestar's Woodcrest)
- Inverse algorithm can absorb 50x increase in CPUs (assuming network keep up with faster processors; granularity will be 70k element/CPU)
- Therefore inverse problem can be solved in 4000\*15hr/400 or ~ 1 week on 8 Pflops machine

#### **Overall remarks:**

- Multilevel continuation forces successive iterates to remain within basin of attraction of global minimum
- Total variation regularization very effective at localizing sharp material interfaces
- Outer and inner iterations are mesh-independent, once nonlinearities have been resolved
- Algorithmic, parallel, and overall scalability follow
- Despite algorithmic and parallel scalability, number of forward/adjoint solutions is large (equivalent to ~800 wave propagations for 129^3 grid)
- Multigrid preconditioner is promising
- High-fidelity inverse earthquake modeling w/multiple earthquake sources remains a petaflops-level challenge

#### Ongoing and future work

- Incorporation of parallel adaptive octree grids
- GCV for regularization parameter selection
- Uncertainty estimation via inverse Hessian
   approximation of covariance matrix
- Incorporation of prior (SCEC community velocity model)
- Inversion for attenuation parameters
- Inversion for fault parameters
- Inversion for fault location (shape optimization problem)

### Acknowledgments

- Ouake Project: Forward/Inverse Earthquake Modeling in Large Basins
   (<u>www.cs.cmu.edu/~quake</u>)
  - o NSF/KDI CMS-9980063, NSF/ITR ATM-0326449
  - o Other Quake group members: Steve Day and Harold Magistrale (SDSU), Jonahan Shewchuk (Berkeley)
- TOPS Center: Toward Optimal Petascale Simulations (www.tops-scidac.org)
  - o Supported under DOE SciDAC program
  - o Collaboration with LLNL, ANL, LBNL, SNL + 5 universities
- Caliente Project: Dynamic Inversion and Control

(www.cs.cmu.edu/~caliente)

- o NSF/ITR ACI-0121667
- o Collaborators: Larry Biegler (CMU), David Keyes (Columbia), Matthias Heinkenschloss (Rice), Roscoe Bartlett, Kevin Long, and Bart van Bloemen Waanders (Sandia), David Young (Boeing), Frank Fendell (TRW)
- DDDAS Project: Real-time Inversion, Prediction, and Sensor Steering
  - o NSF/CNS-0540372
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Kallivokas



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Leonardo Ricardo Taborda Ramirez-Guzman



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