CARP-CG: a computational study

Art Petrenko, December 4, 2012

SLIM
University of British Columbia

Motivation

- Full waveform inversion requires many forward solves: $\mathcal{O}(n_f n_s n_{\text{iter}})$
- Since the matrix is very large ($n_x n_y n_z$), direct solvers use too much memory.
- The goal: accelerate an iterative solver.

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Outline

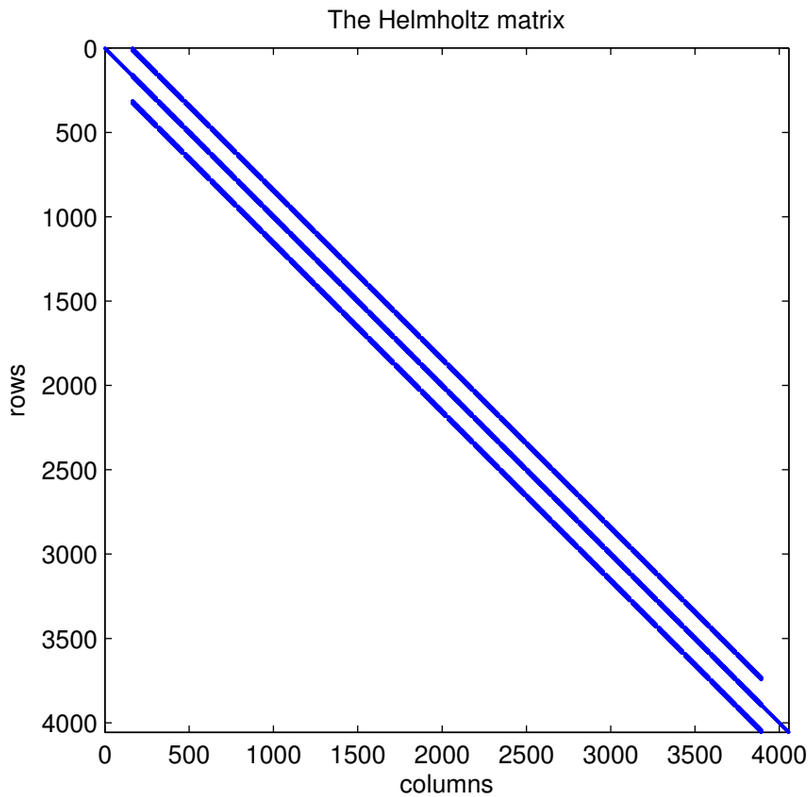
- Problem: solving a linear system
- Algorithm: CARP and CG
- Acceleration: multi-threading
- Performance
- Conclusions

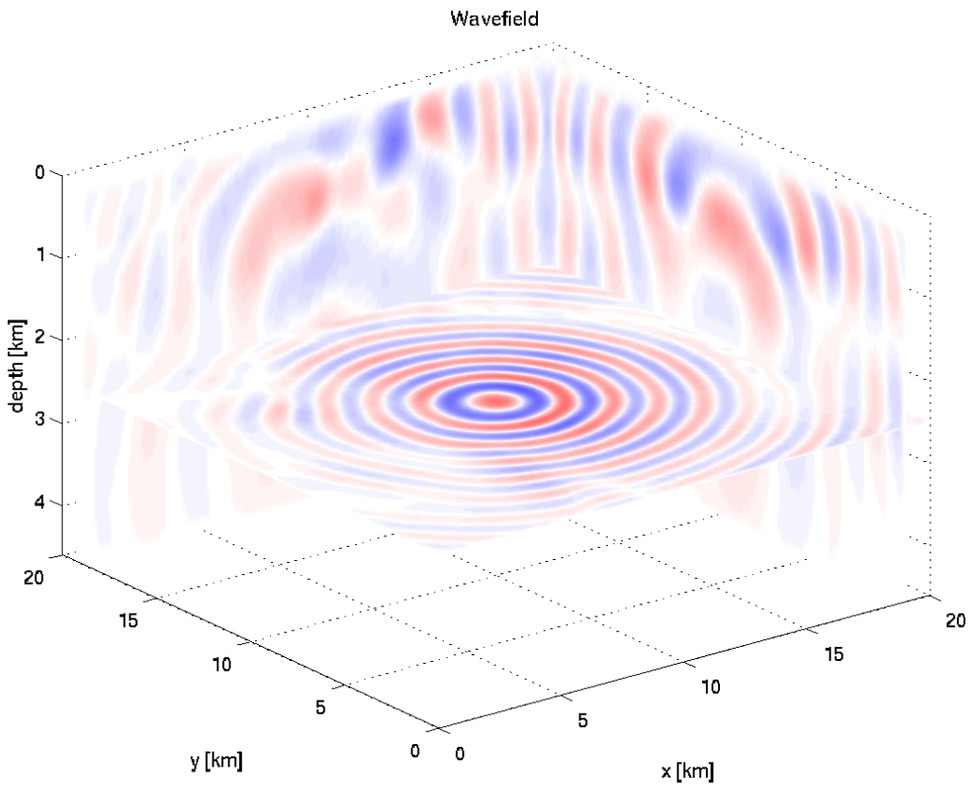
The Helmholtz system

- We solve the constant density (ρ = 1) isotropic acoustic wave equation in the frequency domain:

$$\left(\omega^2\mathbf{m} + \frac{1}{\xi_x(x)}\frac{\partial}{\partial x}\frac{1}{\xi_x(x)}\frac{\partial}{\partial x} + \frac{1}{\xi_y(y)}\frac{\partial}{\partial y}\frac{1}{\xi_y(y)}\frac{\partial}{\partial y} + \frac{1}{\xi_z(z)}\frac{\partial}{\partial z}\frac{1}{\xi_z(z)}\frac{\partial}{\partial z}\right)\mathbf{pressure} = \mathbf{source}$$

$$H\mathbf{u} = \mathbf{q}$$



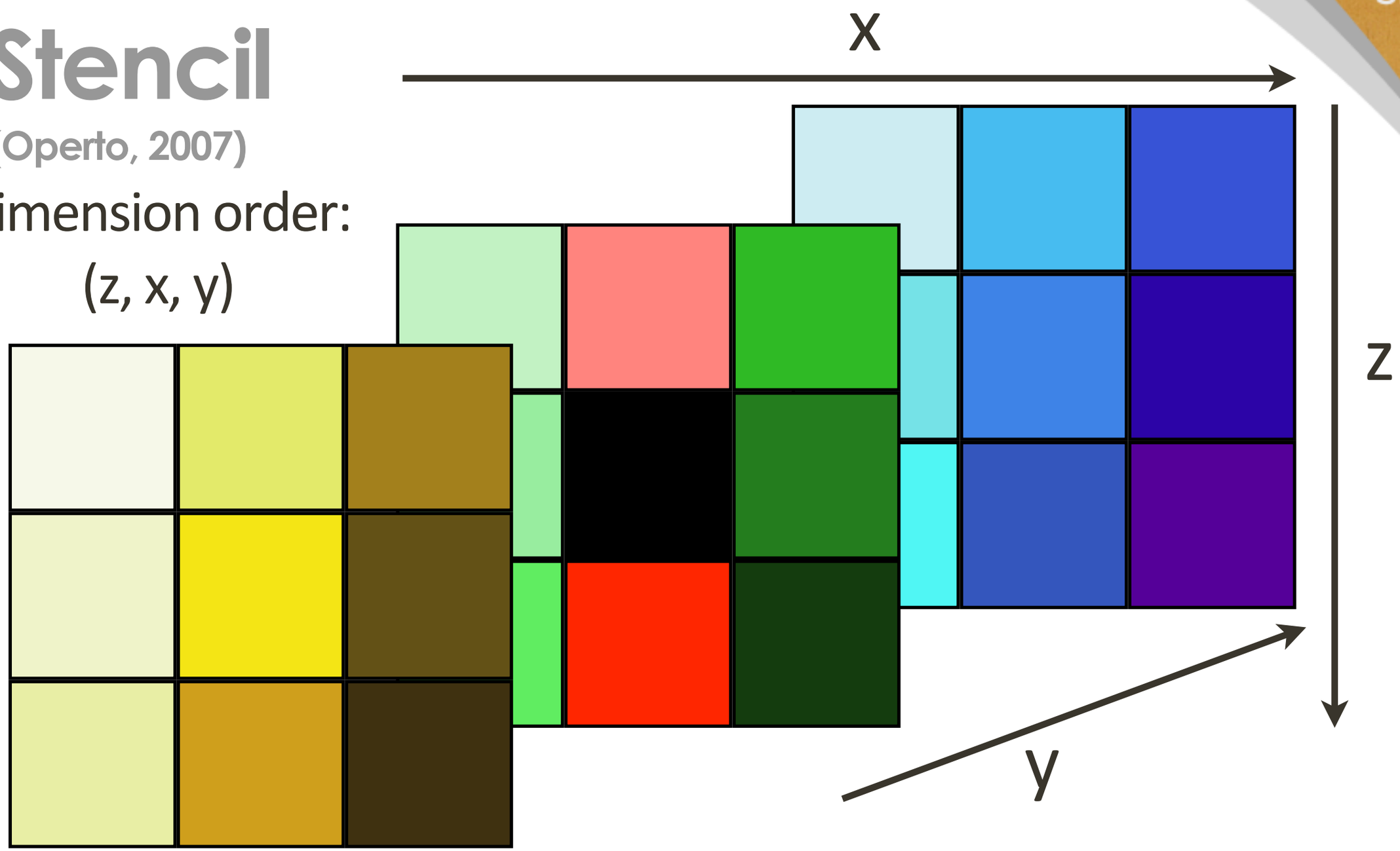


Stencil

(Operto, 2007)

dimension order:

(z, x, y)



Preconditioning needed

- H is not positive definite, hence the method of conjugate gradients is not suitable to solve

$$H\mathbf{u} = \mathbf{q}$$

- We precondition the system into an equivalent, positive definite form:

$$(I - Q)\mathbf{u} = R\mathbf{q}$$

$$A\mathbf{u} = \mathbf{b}$$

- Instead of forming the matrices explicitly, we use the ***double CARP sweep*** operator (Gordon & Gordon, 2005):

$$\mathrm{DCSWP}(H, \mathbf{u}, \mathbf{q}, w) = Q\mathbf{u} + R\mathbf{q}$$

where w is a relaxation parameter.

CARP sweeps explained

- An iterative method for solving generic linear systems.
- The current iterate is projected onto the plane defined by a row of the matrix to become the next iterate:

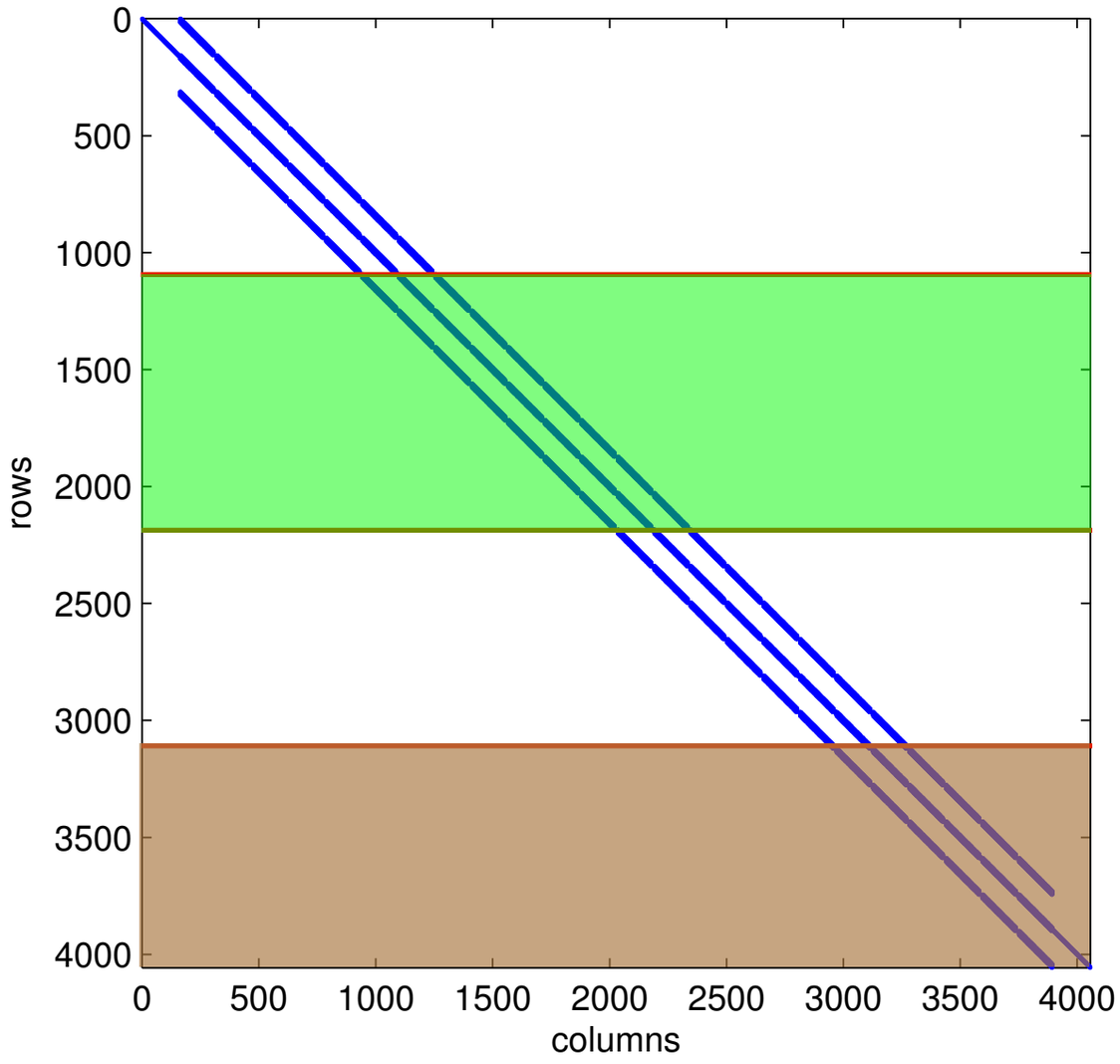
$$\mathbf{u}^{i+1} = \mathbf{u}^i + w(q_k - \mathbf{a}_k \mathbf{u}^i)\mathbf{a}_k^*$$

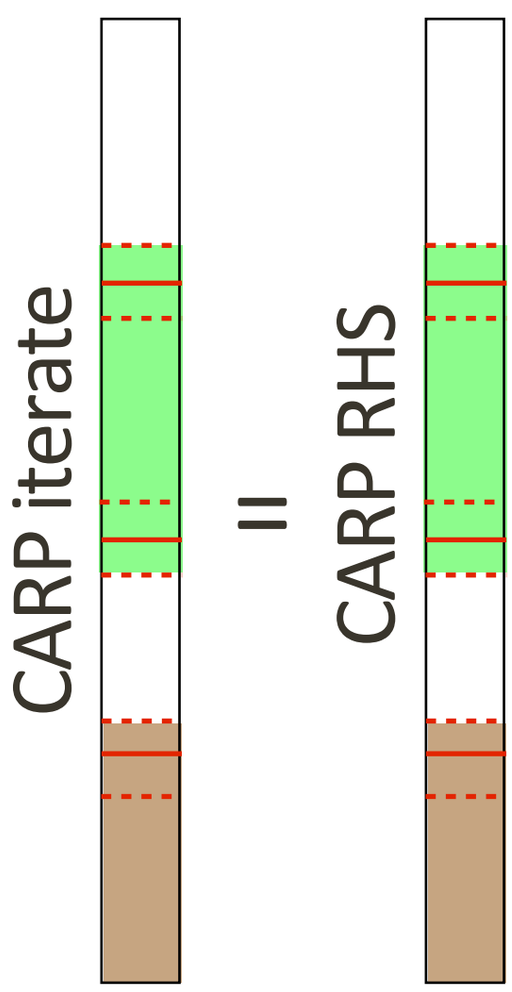
- The matrix rows ($\mathbf{a}_k$) are divided into possibly overlapping sets which undergo the algorithm in ***parallel.***
- Iterate ($\mathbf{u}^i$) elements shared between sets are averaged.
- Index during double sweep:

$$k : 1 \rightarrow N \rightarrow 1$$

Parallelization

The Helmholtz matrix





nodes or threads

The CARP-CG algorithm

(Gordon & Gordon, 2010)

Vanilla CG

Input: H, $\mathbf{u^0}$, $\mathbf{q}$

$i = 0$

$\mathbf{r}^0 = \mathbf{q} - H\mathbf{u}^0$

$\mathbf{p}^0 = \mathbf{r}^0$

while $\left\|\mathbf{r}^i\right\|^2 > tol$ **do**

$\mathbf{q}^i_{cg} = H\mathbf{p}^i$

$\alpha = \left\|\mathbf{r}^i\right\|^2 / \left\langle \mathbf{p}^i, \mathbf{q}^i_{cg} \right\rangle$

$\mathbf{u}^{i+1} = \mathbf{u}^i + \alpha \mathbf{p}^i$

$\mathbf{r}^{i+1} = \mathbf{r}^i - \alpha \mathbf{q}^i_{cg}$

$\beta = \left\|\mathbf{r}^{i+1}\right\|^2 / \left\|\mathbf{r}^i\right\|^2$

$\mathbf{p}^{i+1} = \mathbf{r}^{i+1} + \beta \mathbf{p}^i$

$i = i + 1$

end while

Output: u

CARP-CG

Input: H, $\mathbf{u^0}$, $\mathbf{q}$, w

$i = 0$

$\mathbf{b} = \mathrm{DCSWP}(H, \mathbf{0}, \mathbf{q}^0, w)$

$\mathbf{r}^0 = \mathbf{b} - \mathbf{u}^0 + \mathrm{DCSWP}(H, \mathbf{u}^0, \mathbf{0}, w)$

$\mathbf{p}^0 = \mathbf{r}^0$

while $\left\|\mathbf{r}^i\right\|^2 > tol$ **do**

$\boldsymbol{tmp} = \mathrm{FCSWP}(H, \mathbf{p^i}, \mathbf{0}, w)$

$\mathbf{q}^i_{cg} = \mathbf{p}^i - \mathrm{BCSWP}(H, \boldsymbol{tmp}, \mathbf{0}, w)$

$\alpha = \left\|\mathbf{r}^i\right\|^2 / \left\langle \mathbf{p}^i, \mathbf{q}^i_{cg} \right\rangle$

$\mathbf{u}^{i+1} = \mathbf{u}^i + \alpha \mathbf{p}^i$

$\mathbf{r}^{i+1} = \mathbf{r}^i - \alpha \mathbf{q}^i_{cg}$

$\beta = \left\|\mathbf{r}^{i+1}\right\|^2 / \left\|\mathbf{r}^i\right\|^2$

$\mathbf{p}^{i+1} = \mathbf{r}^{i+1} + \beta \mathbf{p}^i$

$i = i + 1$

end while

Output: u

Implementation

- **CG:** MATLAB
- **CARP sweep:** C source compiled into MEX file that is called from MATLAB like a function.
- CARP source:

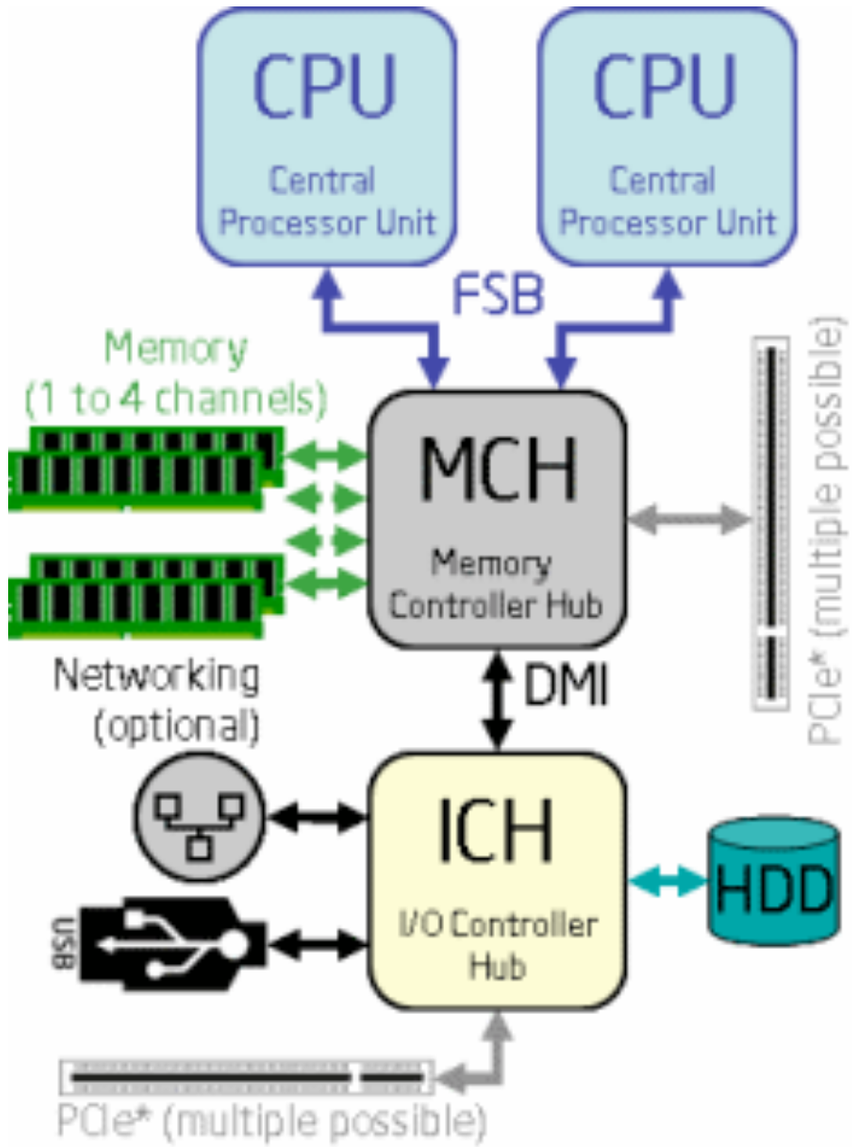
```
for(i=0;i<nrow;i++){
    cr = br[i+(int)idx[idx_mid]];
    ci = bi[i+(int)idx[idx_mid]];
    for(j=0;j<ncol;j++){
        k = i + (int)idx[j];
        if(k>=0 && k<nx){
            cr -= Sr[i*ncol + j]*yr[k] - Si[i*ncol + j]*yi[k];
            ci -= Sr[i*ncol + j]*yi[k] + Si[i*ncol + j]*yr[k];
        }
    }
    cr *= w;
    ci *= w;
    for(j=0;j<ncol;j++){
        k = i + (int)idx[j];
        if(k>=0 && k<nx){
            yr[k] +=   cr*Sr[i*ncol + j] + ci*Si[i*ncol + j];
            yi[k] +=  -cr*Si[i*ncol + j] + ci*Sr[i*ncol + j];
        }
    }
}
```

Implementation details

- Helmholtz matrix is sparse and structured; it is stored as rows of non-zero diagonals and their offsets.
- Row-wise storage of diagonals ensures memory is accessed sequentially.
- pthreads library used for multi-threading.
- gcc with the -O option used for compilation.
- Also tried -O2 -O3, difference of less than 5% in timing.
- Single-threaded FORTRAN sweeps implemented, but were slower than C.

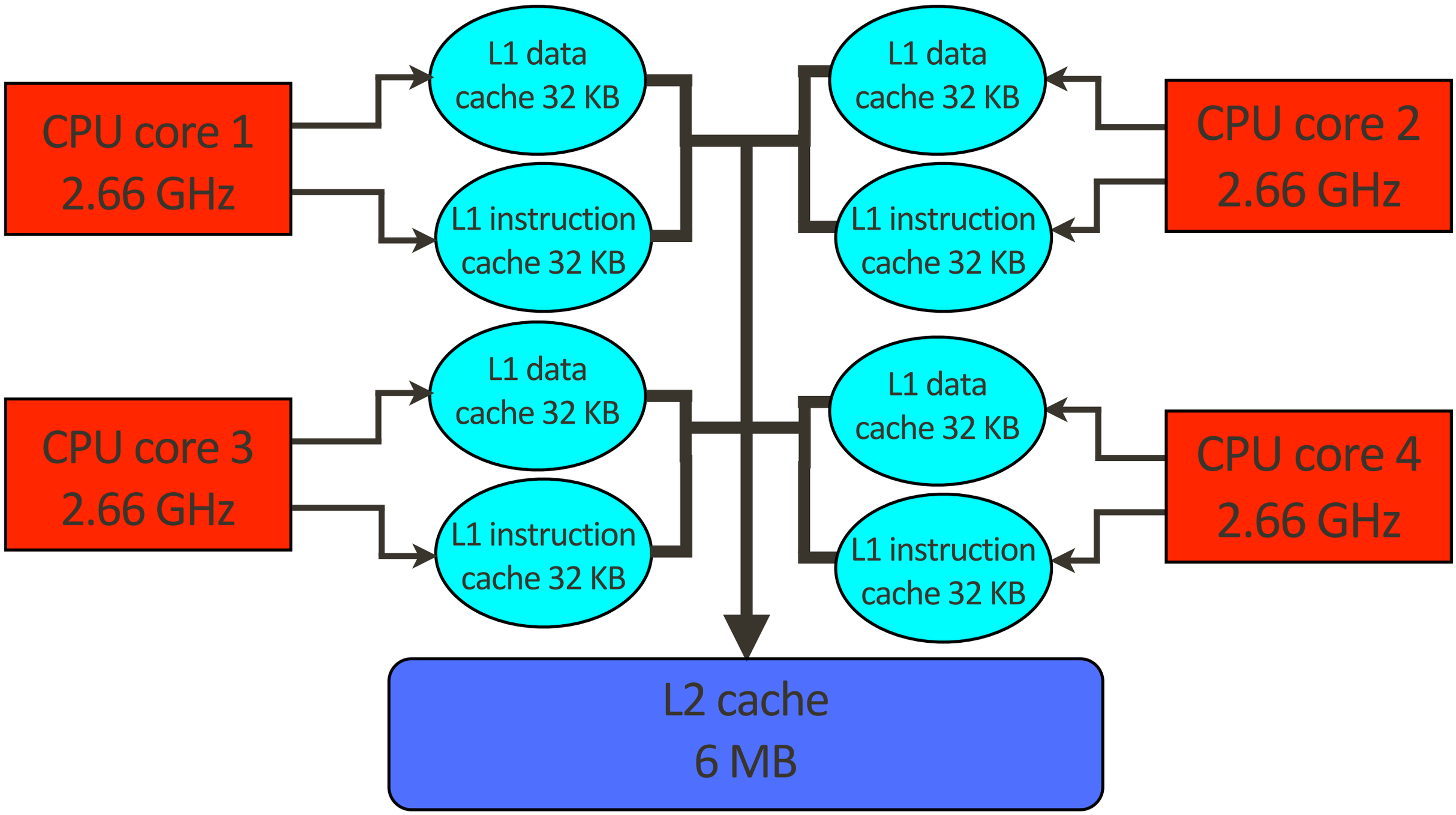
LIMA cluster node

- Intel Xeon E5430 quad core, dual CPU
- Each CPU has its own Front Side Bus for communication with memory



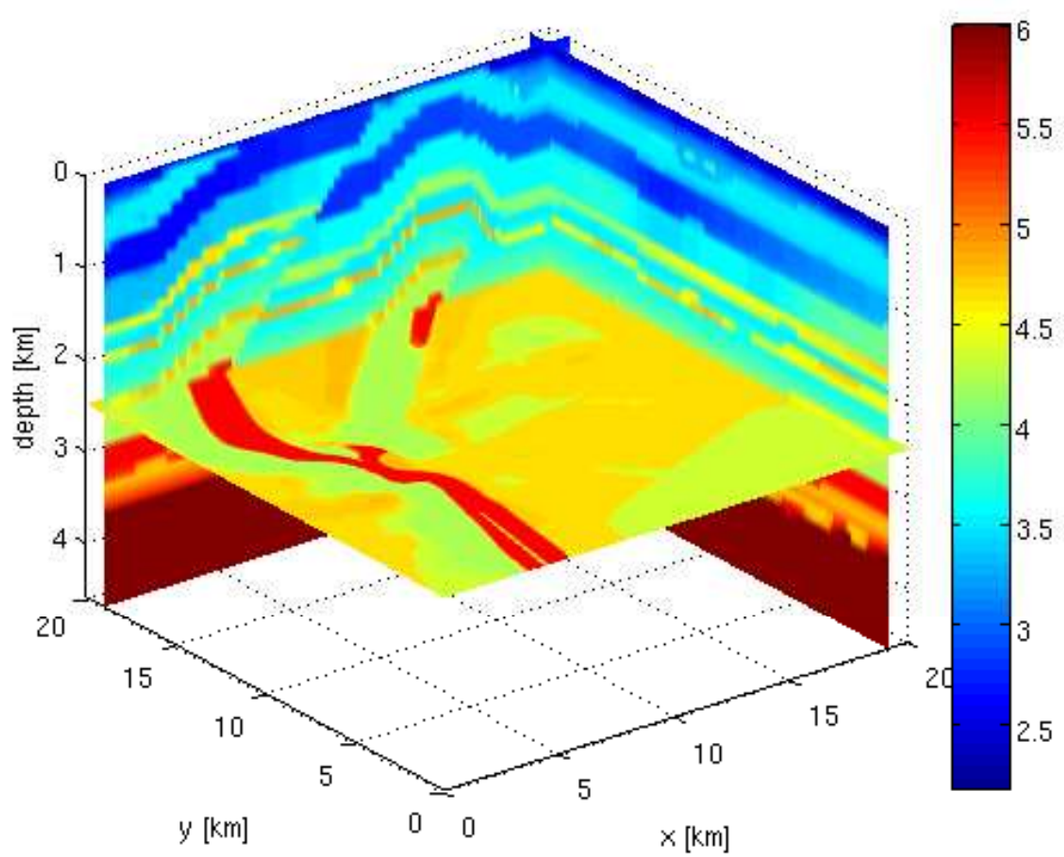
source: http://ark.intel.com/products/33081/Intel-Xeon-Processor-E5430-12M-Cache-2_66-GHz-1333-MHz-FSB

Intel Xeon E5430 layout

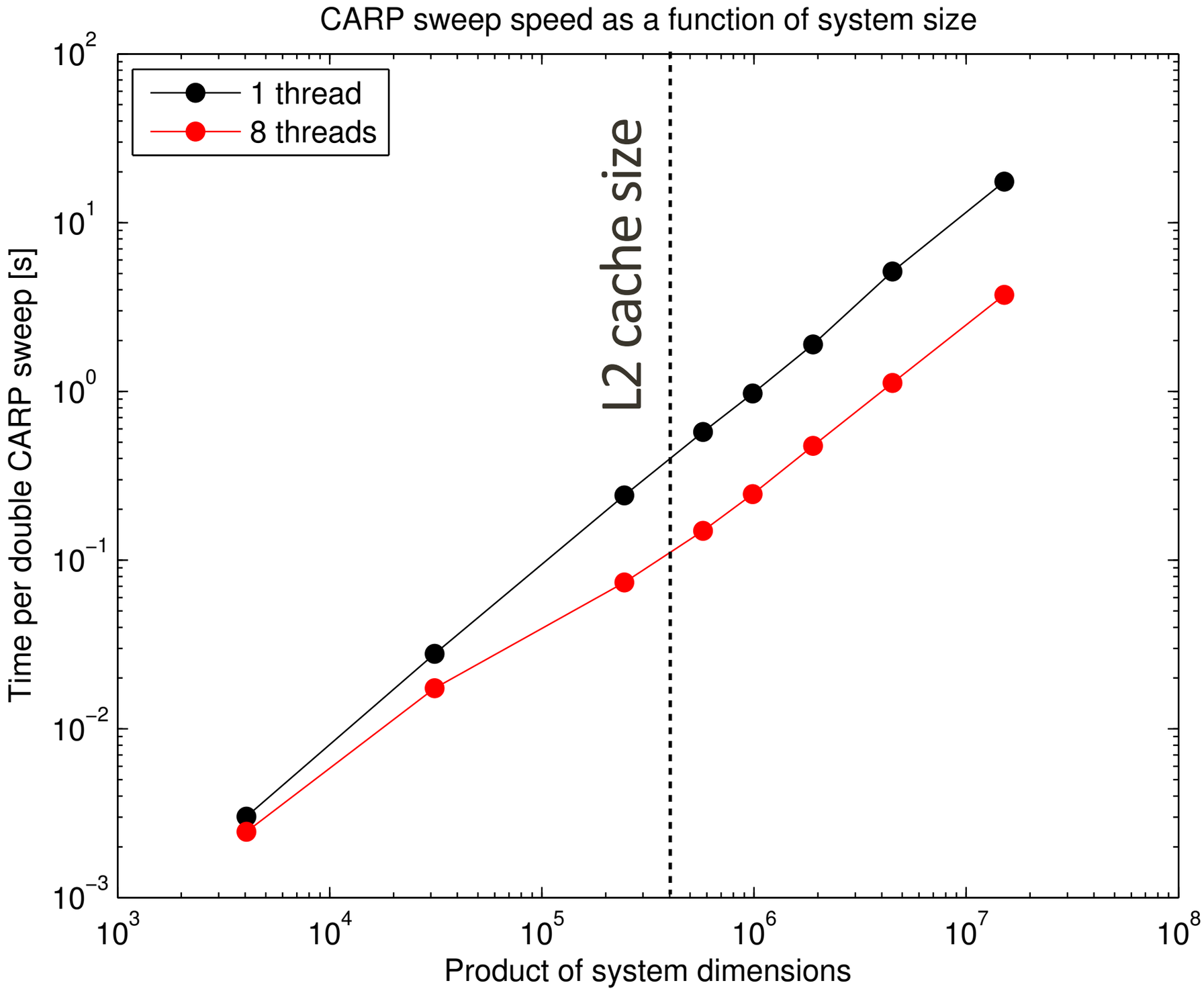


CARP Experiment set-up

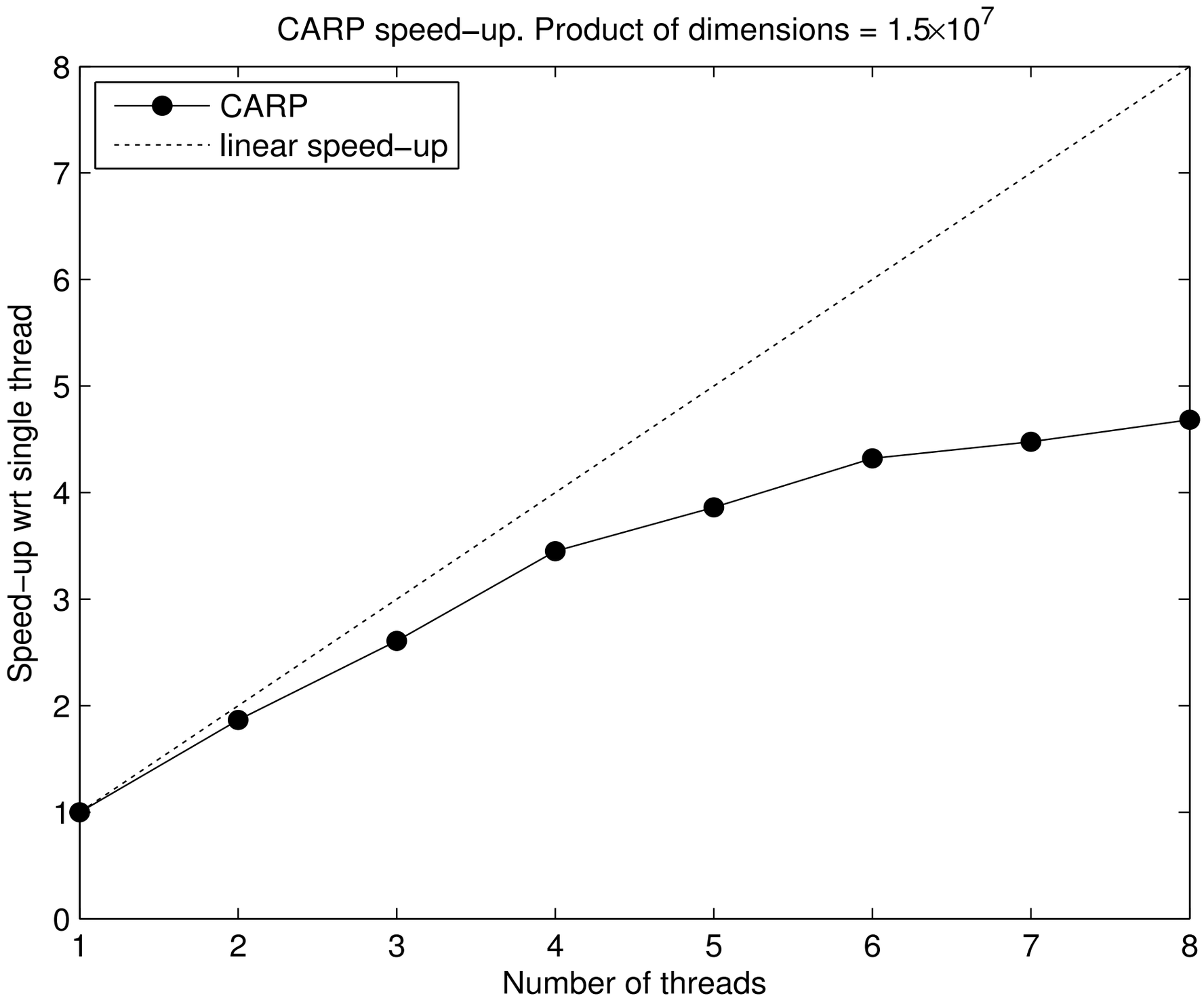
- SEG/EAGE Overthrust model, under-sampled with factors of 2—6, 8, 16, 32.
- Simultaneous source throughout the domain, with normally distributed amplitude.
- w = 1.5
- Zero initial guess.
- Timings are per one CARP double sweep.
- Timings of five runs are averaged for each combination of (system size, degree of parallelism)
- Frequency = 12 Hz / under-sampling



Timing CARP


CARP sweep speed as a function of system size
1 thread
8 threads
L2 cache size
Time per double CARP sweep [s]
Product of system dimensions
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{3}
10^{4}
10^{5}
10^{6}
10^{7}
10^{8}

Timing CARP: speed-up

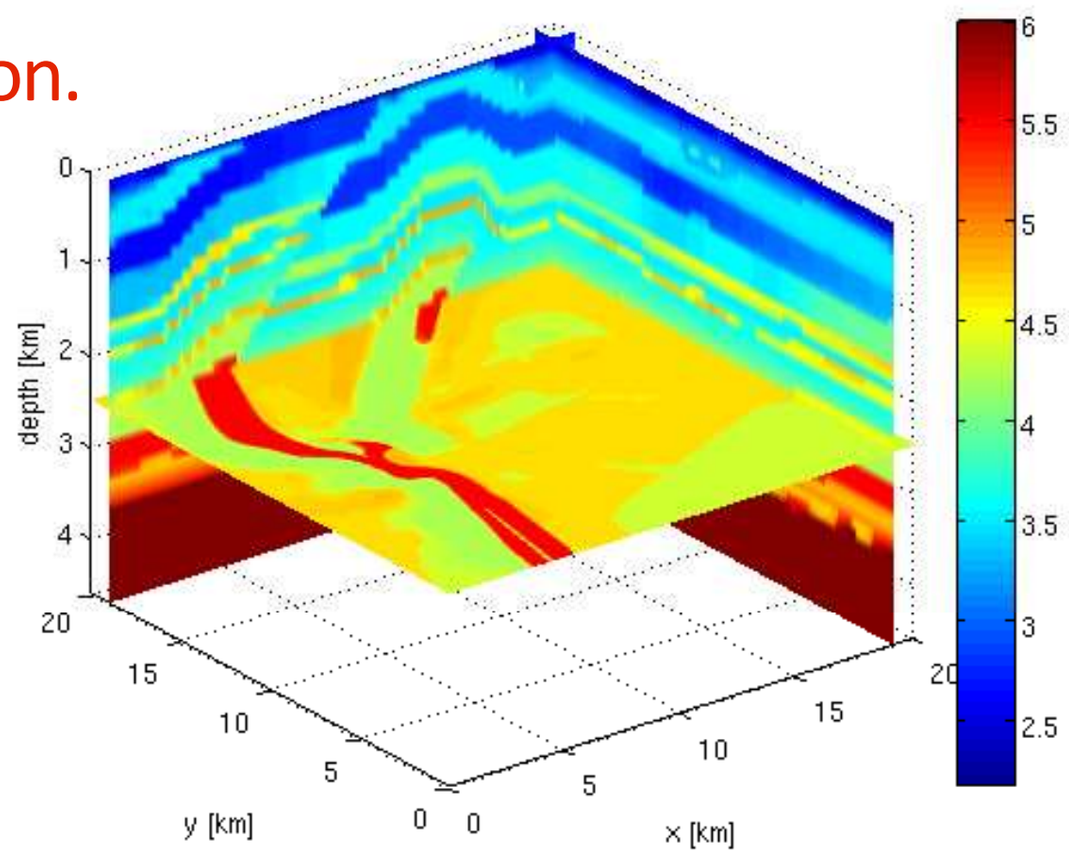


On to CARP-CG: Distributed or shared memory?

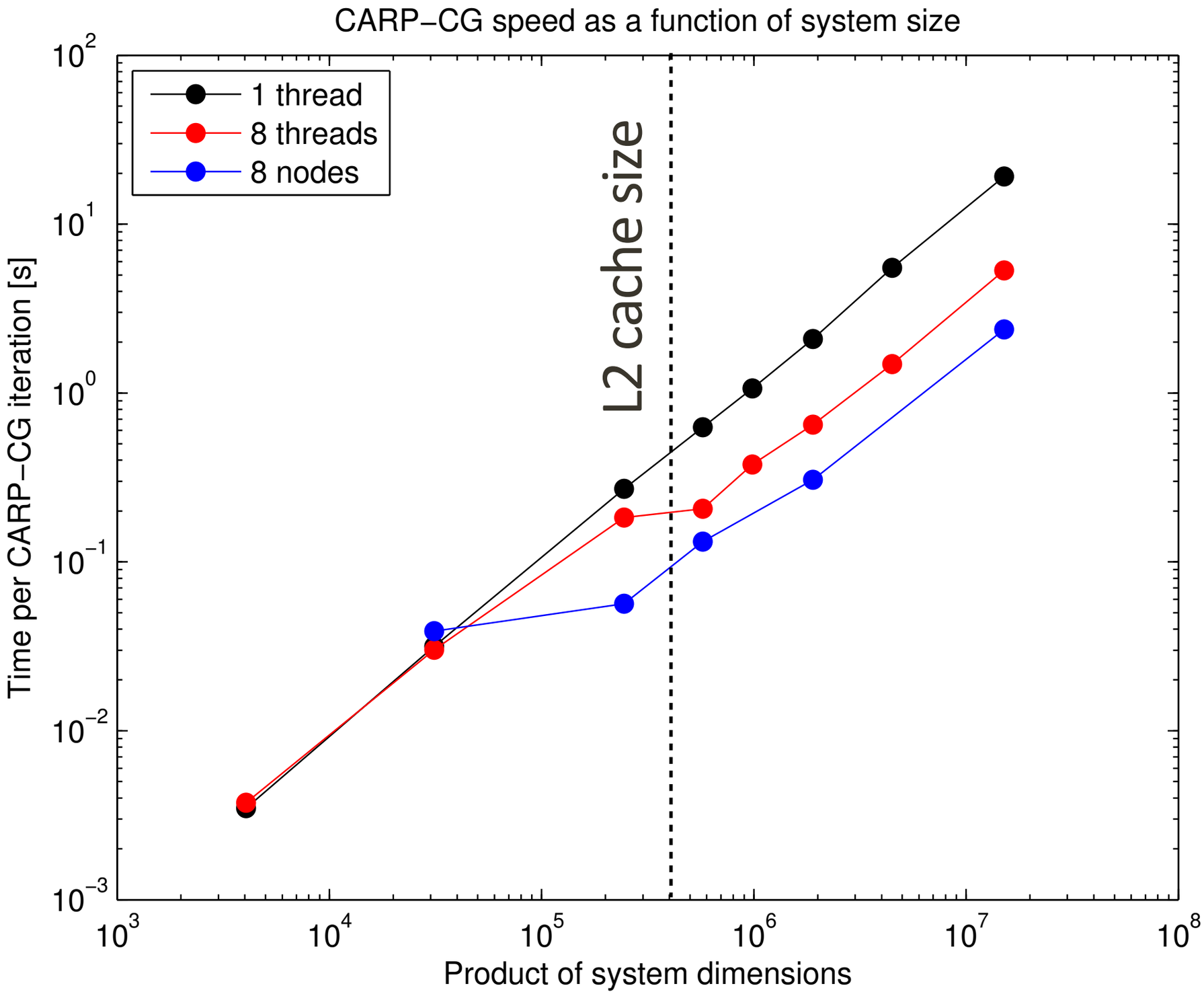
- Distributed setup (parallelization over nodes) has expensive inter-node communication.
- Shared setup (parallelization over threads) has bottle-necks at the cache, memory controller, and memory bus.

CARP-CG Experiment set-up

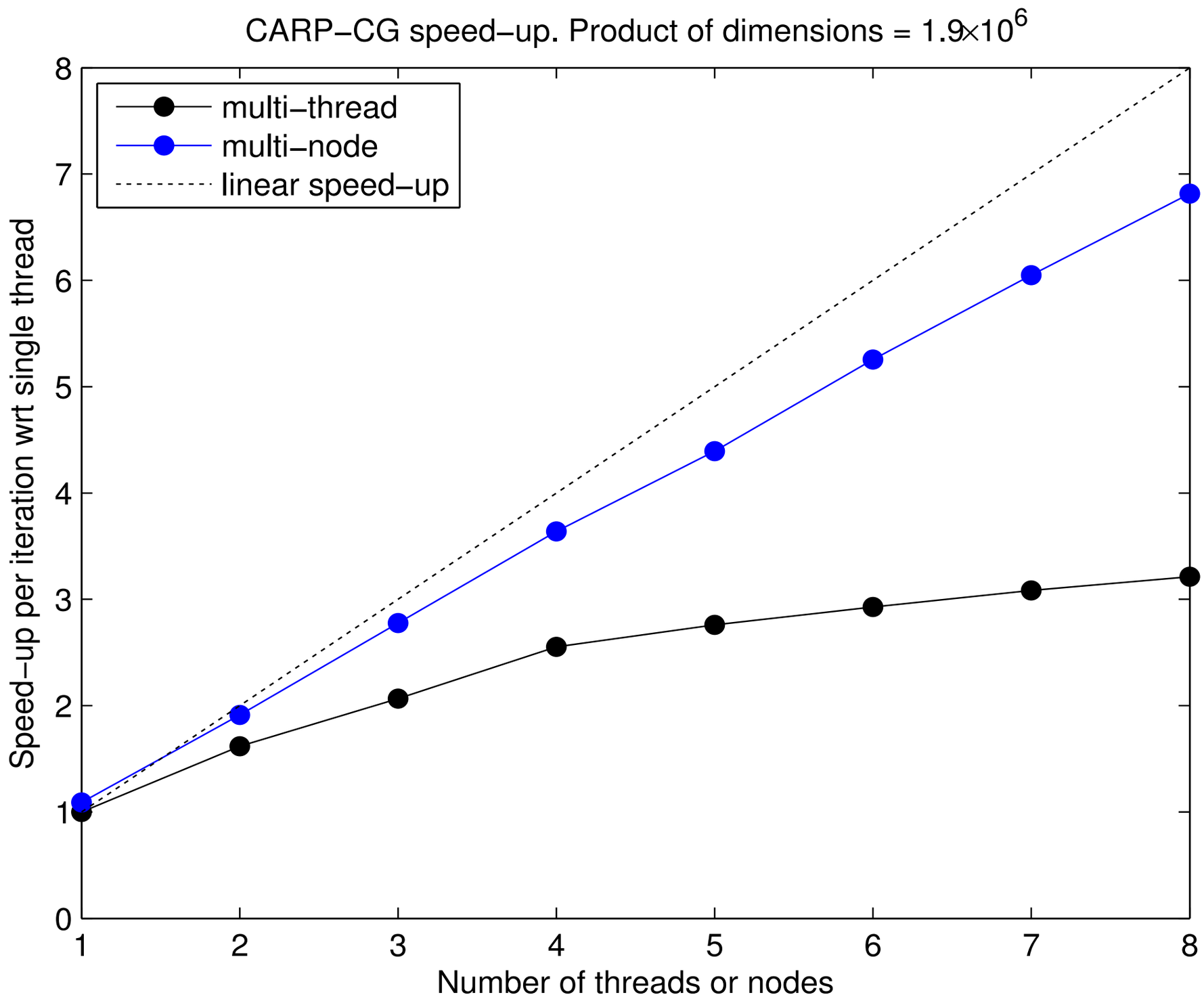
- SEG/EAGE Overthrust model, under-sampled with factors of 2—6, 8, 16, 32.
- Simultaneous source throughout the domain, with normally distributed amplitude.
- w = 1.5
- Zero initial guess.
- Timings are per one CARP-CG iteration.
- CARP-CG converges to a tolerance of 10^{-4}.
- Timings of five runs are averaged for each combination of (system size, degree of parallelism)
- Frequency = 12 Hz / under-sampling



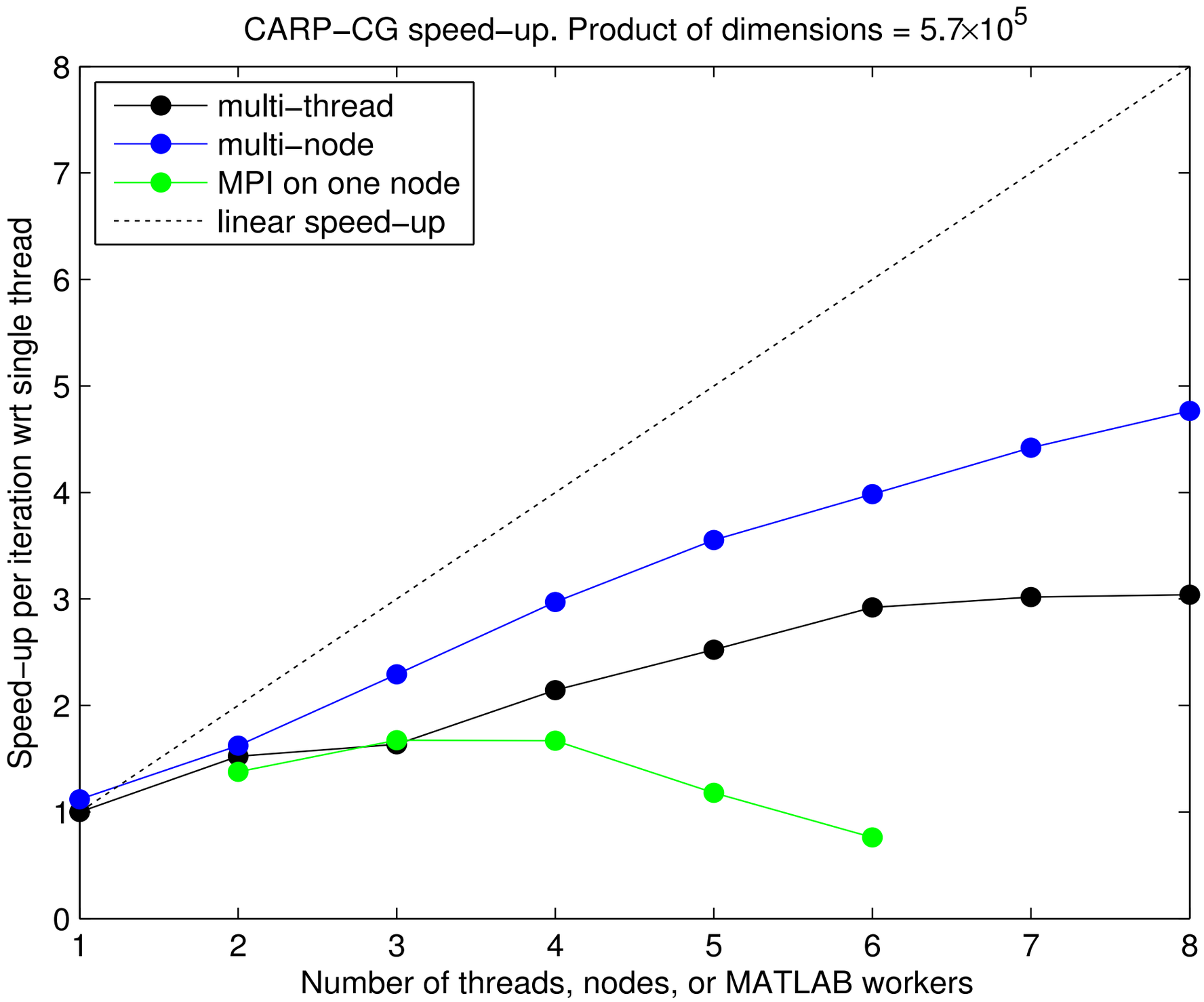
Nodes vs. Threads



Nodes vs. Threads



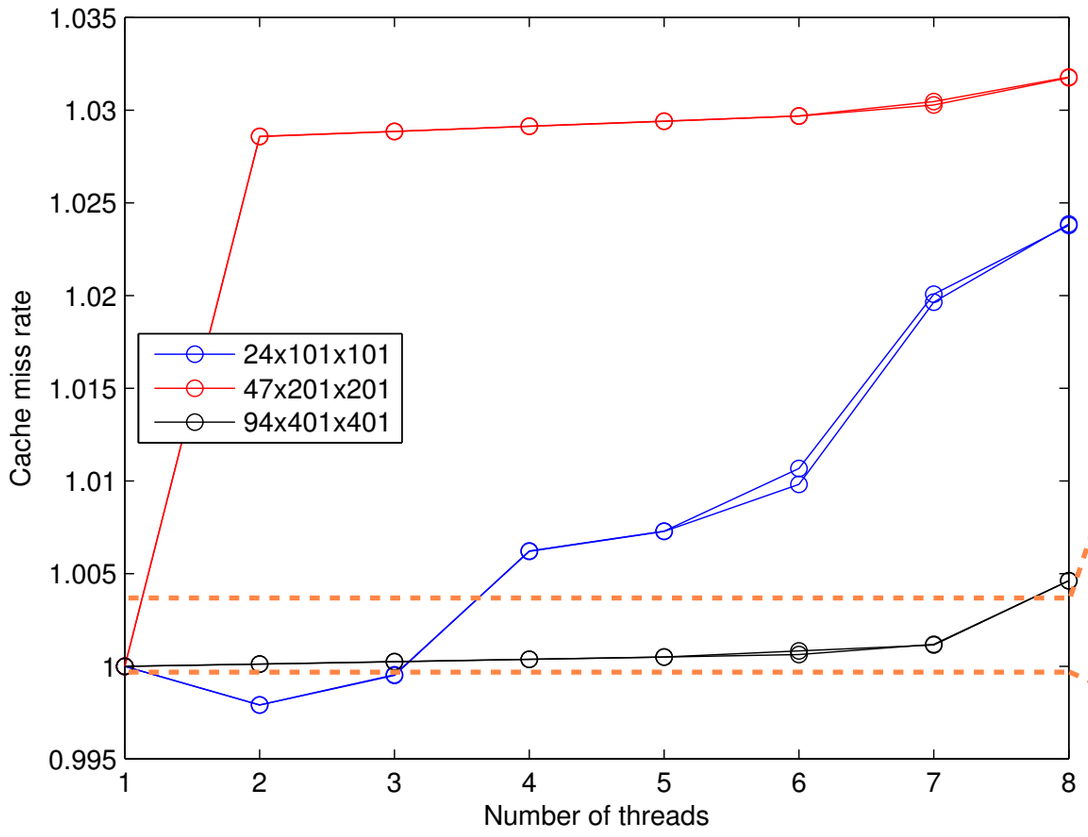
Nodes vs. Threads



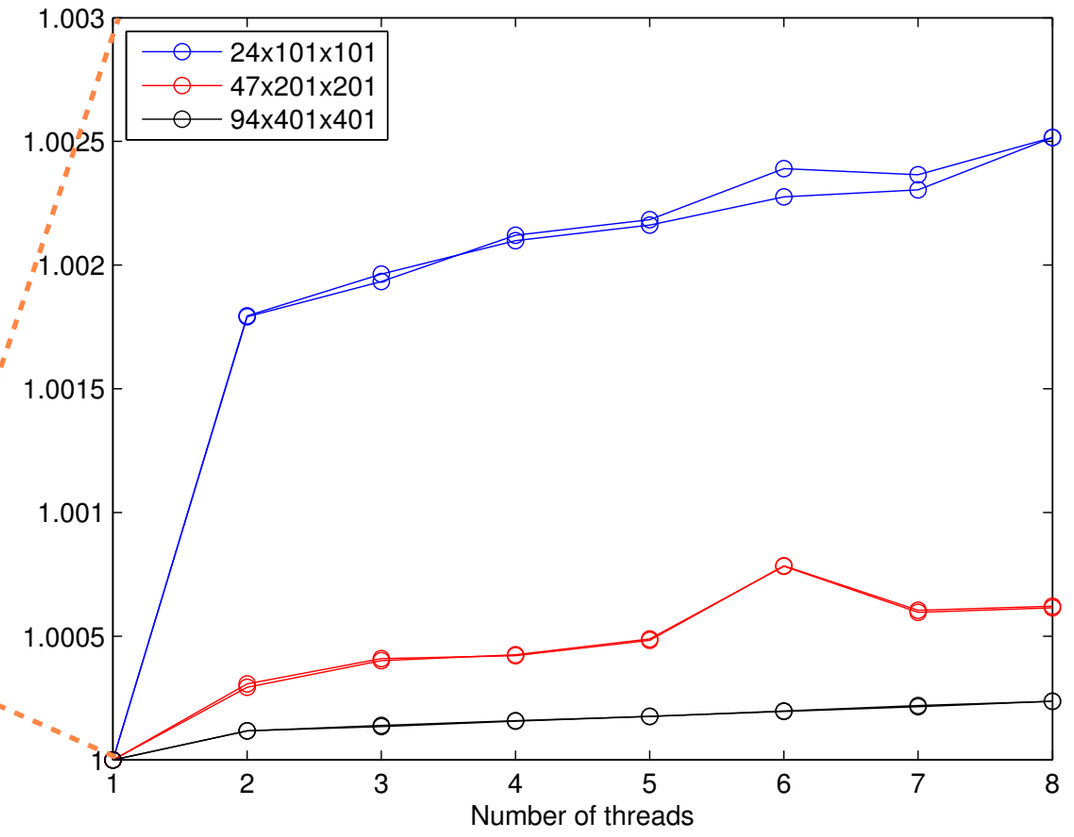
Measuring cache misses

- One forward CARP sweep
- SEG/EAGE overthrust model
- zero initial guess, normally distributed source
- valgrind --tool=cachegrind --fair-sched=yes

L2 cache misses



L1 cache misses



Conclusions and obvious improvements

- Cache misses are not the main reason for slow performance of threaded CARP sweeps.
- Combine MPI across several nodes with multi-threading on each node.
- All of CARP-CG will be re-written in C/MEX (complete), threaded (in progress) and MPI implemented (to be done).
- Intel compiler will be used for finer tuning of the sweeps to the E5430 Xeon chip.

The Future: CARP-CG on Maxeler's Dataflow Engine

- Dataflow models computing as operations on a stream.
- Rather than executing instructions in ***time***, they are laid out in ***space*** on an FPGA.
- After the initial latency, output is one element per clock cycle.
- Even with the large (68 GB/s) memory bandwidth, the problem will still be memory bound.
- To partially alleviate the situation, the Helmholtz matrix can be computed on the fly.
- Based on initial estimates, we anticipate a speed-up of the order of 100.

Acknowledgements

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SINBAD

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Selected references

- **Operto et al. 2007**: Stéphane Operto, Jean Virieux, Patrick Amestoy, Jean-Yves L'Excellent, Luc Giraud and Hafedh Ben Hadj Ali. *3D finite-difference frequency-domain modeling of visco-acoustic wave propagation using a massively parallel direct solver: A feasibility study*. Geophysics 72(5).
- **Gordon & Gordon 2005:** *Component-Averaged Row Projections: A Robust, Block-Parallel Scheme for Sparse Linear Systems*. SIAM J. Sci. Computing 27(3).
- **Gordon & Gordon 2010:** *CARP-CG: A robust and efficient parallel solver for linear systems, applied to strongly convection dominated PDEs*. Parallel Computing 36.
- **van Leeuwen, Gordon & Gordon and Herrmann 2012**: *Preconditioning the Helmholtz equation via row-projections.* EAGE Conference.

MATLAB vs. julia