# Performance of time and frequency domain cluster solvers compared to geophysical applications

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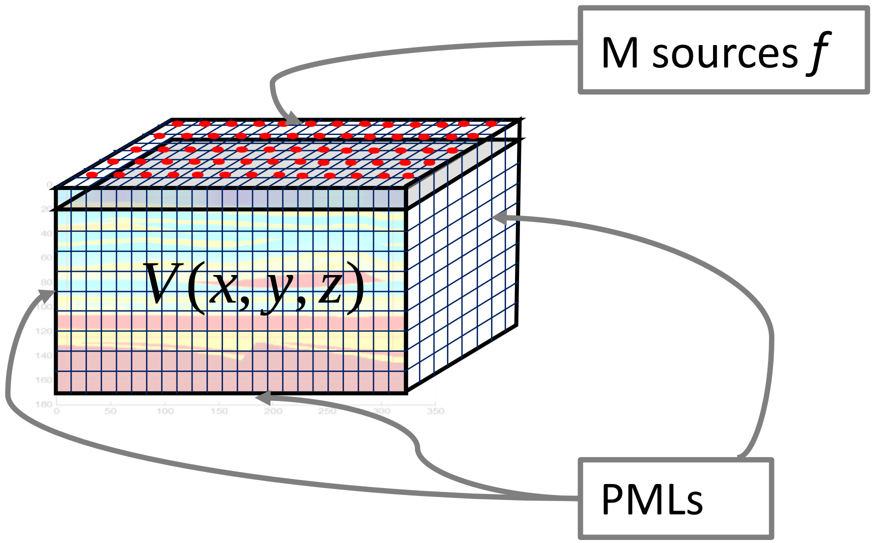
where energy is opportunity

# Agenda

1. Problem setting
2. Acoustic wavefield simulations: Time and frequency domain approaches
3. Numerical experiments: Comparison of proposed approaches

# Problem setting




Full Waveform Inversion (FWI) in frequency domain for macro velocity reconstruction.

Acoustic wavefield simulations:

- Set of frequencies [1,15] Hz
- Many sources (> 10 000)

Direct acoustic problem, two approaches:

- Time-domain
- Frequency-domain (our choice)

# Acoustic wavefield simulations

## Time-domain (TD):

- Wave equation

$$\frac{\partial^2 p}{\partial t^2} - V^2(x,y,z)\Delta p = f(t)\delta(x - x_s, y - y_s, z - z_s)$$

- Apply Fourier transform

$$\hat{p}(\omega, x, y, z) = \int e^{-i\omega t} p(t, x, y, z) dt$$

## Frequency-domain (FD)

- Helmholtz equation

$$\Delta u + \frac{\omega^2}{V^2(x,y,z)} u = \delta(x - x_s, y - y_s, z - z_s)$$

- Direct solver (our choice)

# Acoustic wavefield simulations

## Time-domain (TD):

- Wave equation

$$\frac{\partial^2 p}{\partial t^2} - V^2(x,y,z)\Delta p = f(t)\delta(x - x_s, y - y_s, z - z_s)$$

- Apply Fourier transform

$$\hat{p}(\omega, x, y, z) = \int e^{-i\omega t} p(t, x, y, z) dt$$

✓ Low memory consumption

✓ Easy parallelization: 1 shot per 1 node

## Frequency-domain (FD)

- Helmholtz equation

$$\Delta u + \frac{\omega^2}{V^2(x,y,z)} u = \delta(x - x_s, y - y_s, z - z_s)$$

- Direct solver (our choice)

✓ Direct solvers are efficient for many sources.

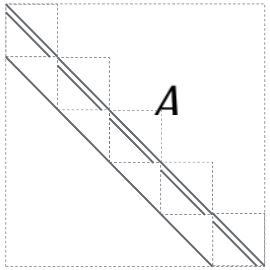
## Benefits

# Frequency-domain: Direct solver outline

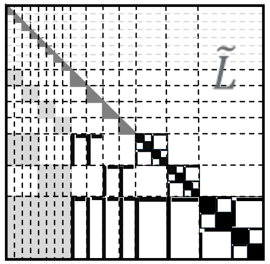
- Finite Difference approximation
- Optimal 27-point stencil
- Perfectly Matched Layers (PMLs)

$$AU = F$$

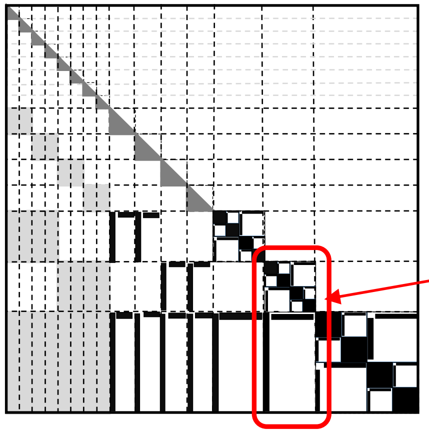
- ✓ $LDL^t$- matrix decomposition
- ✓ Nested Dissection (ND) reordering
- ✓ Low-Rank approximation; Hierarchically Semi Separable (HSS) format



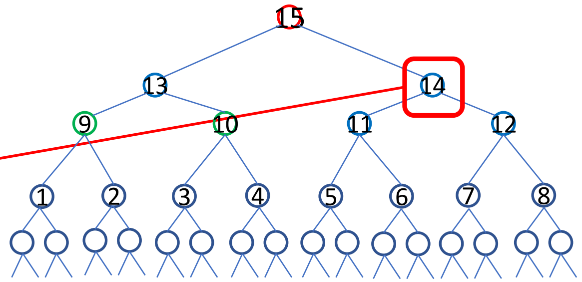

$$\hat{A} = PAP^t;\ \hat{A} \cong \tilde{L}\tilde{D}\tilde{L}^t$$



# Parallelization (LDLt-factorization and solve LDLtU=F step)



Elimination tree (ET) – task dependences




- ✓ Matrix panel distribution amount cluster nodes
- ✓ Compute **Schur** complements and **Low-Rank compression** in parallel (Factorization step)
- ✓ OMP-parallelization within one node; 1 MPI process = 1 cluster node

# Computational time: TD and FD direct solvers

$N_{proc}$ - number of cluster nodes
$N_{shots}$ - number of shots

Time domain solver:

$$T_{TD}(N_{proc}, N_{shots}) = T_{TD}(1,1)\max(\frac{N_{shots}}{N_{proc}}, 1)$$

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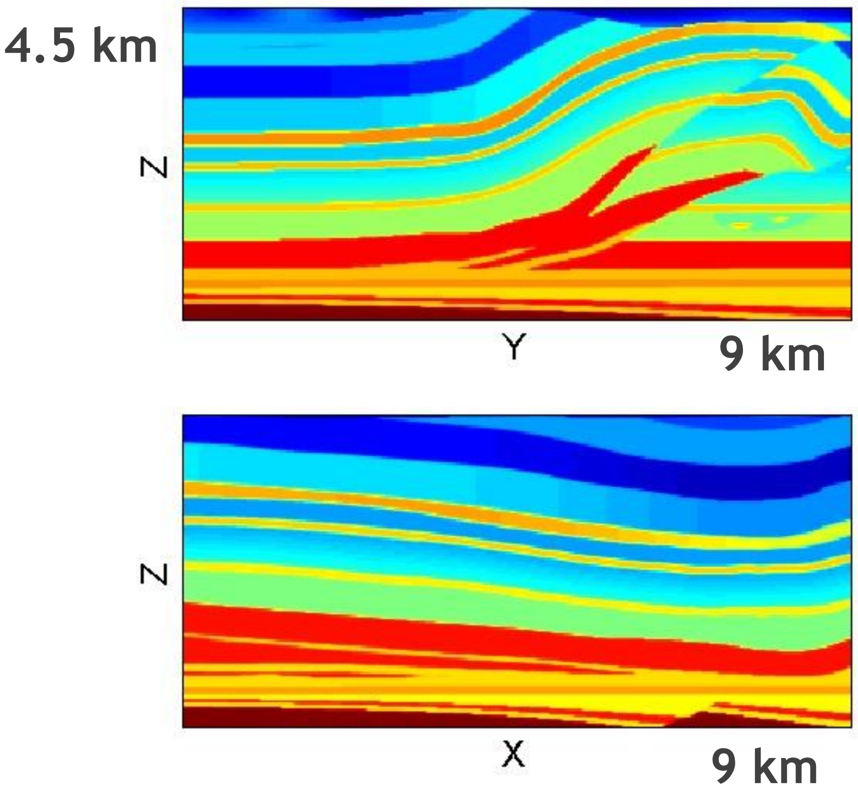
Frequency domain Direct solver:

$$T_{FD}(N_{proc}, N_{shots}) = T_{FCT}(N_{proc}) + T_{SLV}(N_{proc}, 1)N_{shots}$$

# Numerical experiments

# Overthrust (OT) model



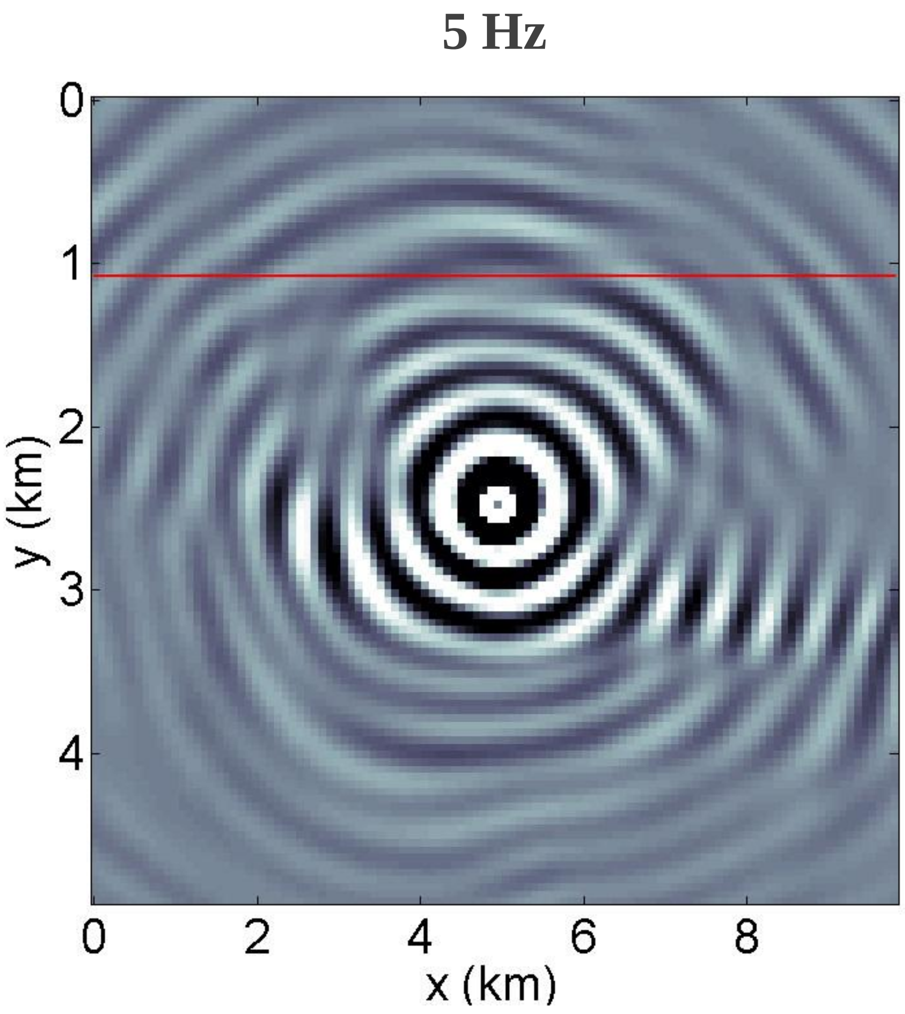

**Model parameters**

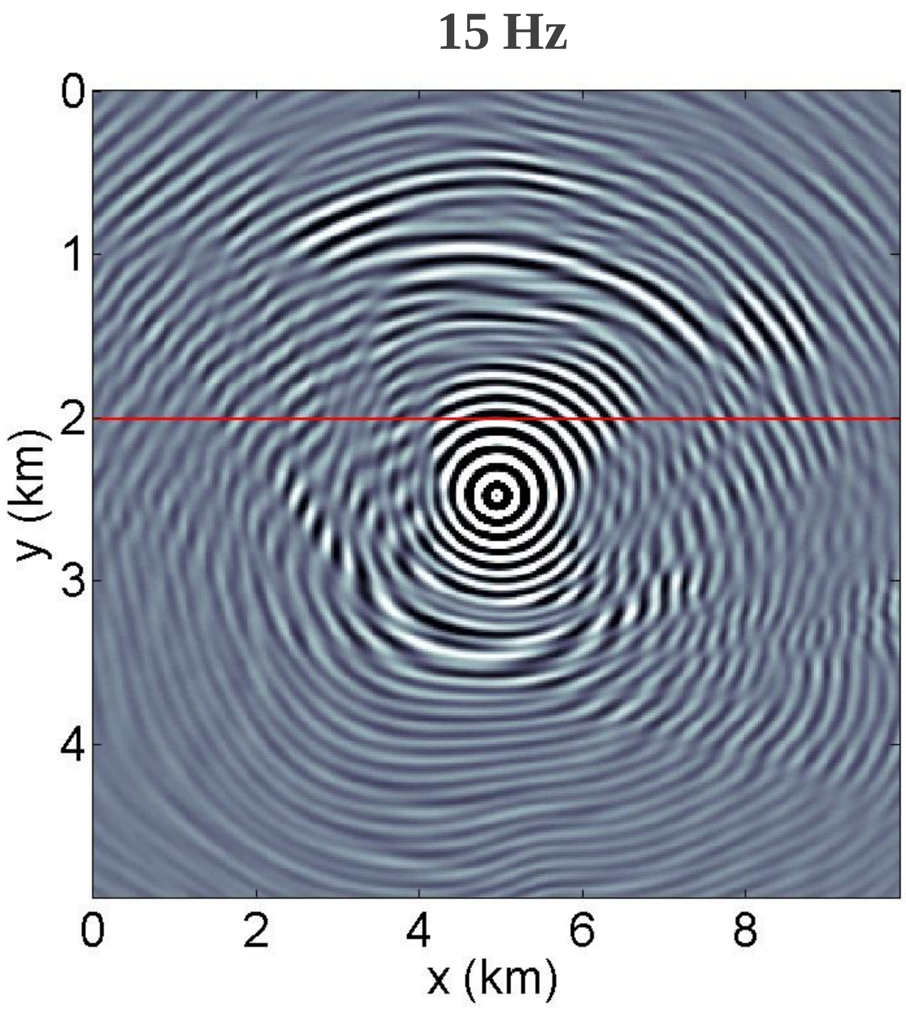
- Physical size: 9 x 9 x 4.5 km
- Mesh step: hx=hy=hz=30m (~17*10^6 unknowns)
- Velocity varies between 2300 m/s and 6000 m/s
- Number of shots $N_{shots}$=12 800
- Frequencies for modeling: 5, 7 and 15 Hz

**Computational resources**:

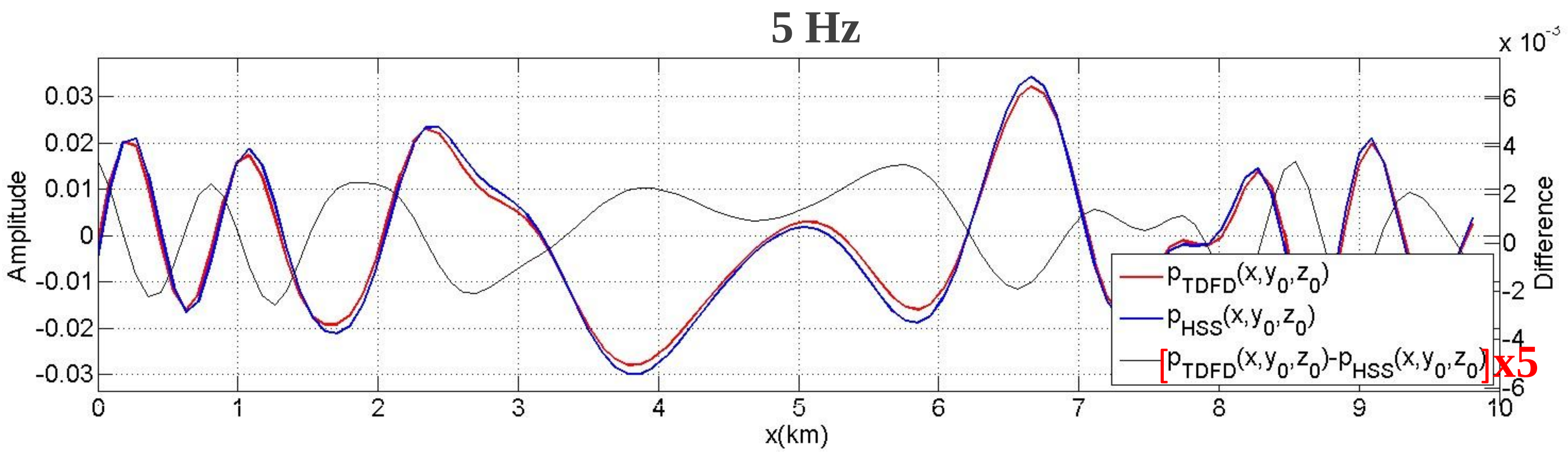
- Shaheen II (2× Intel® Xeon® CPU E5-2698 v3 @2.3 GHz per cluster node, 128 GB RAM/per node)
- 32 cores per node

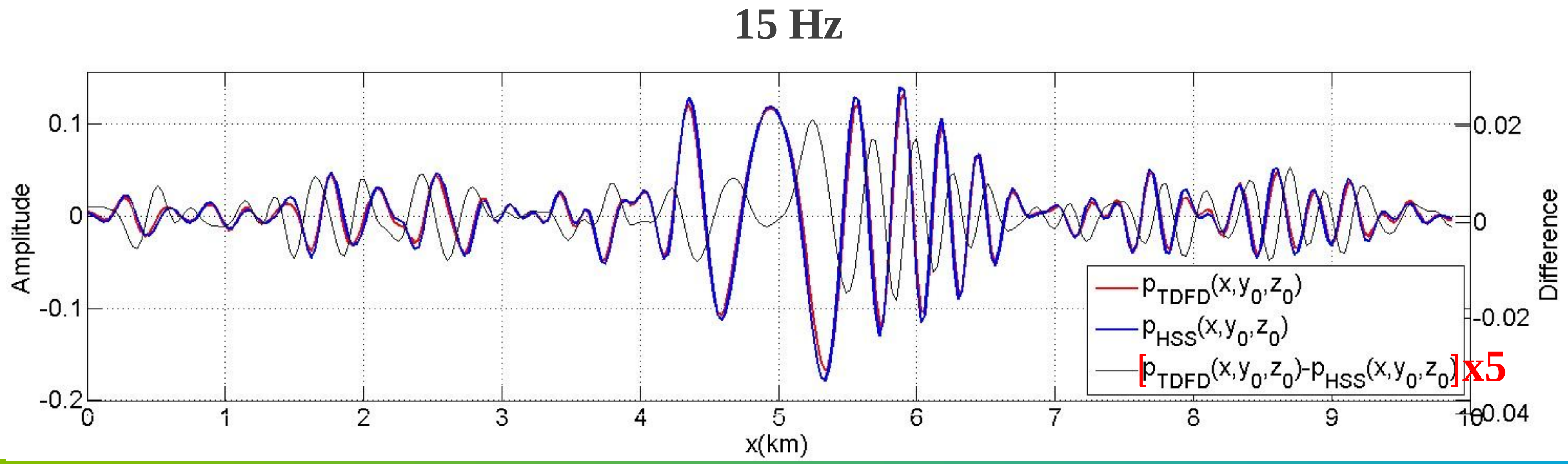
# 2D snapshots of the real part of the computed wavefield



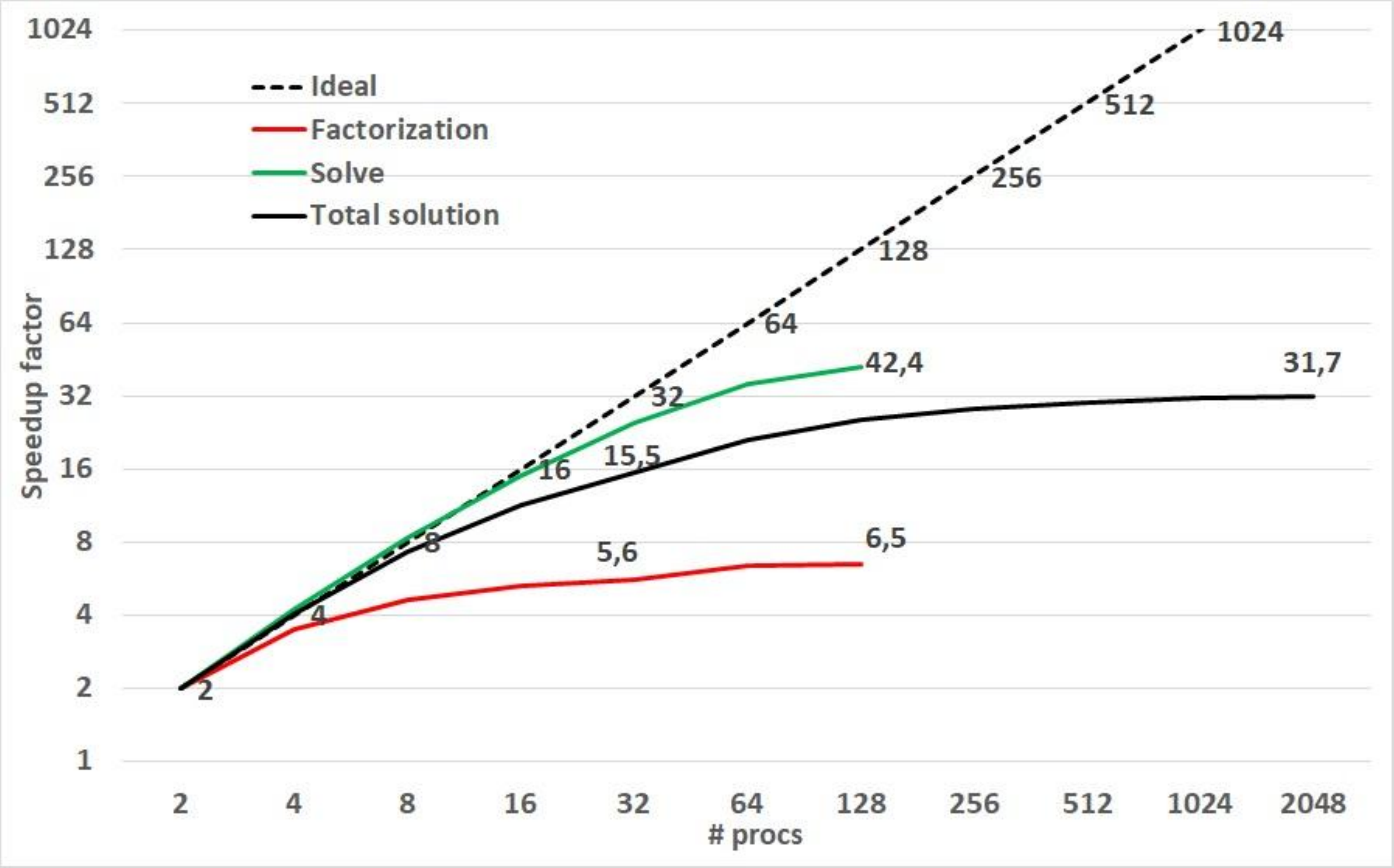



# Solutions along selected profiles

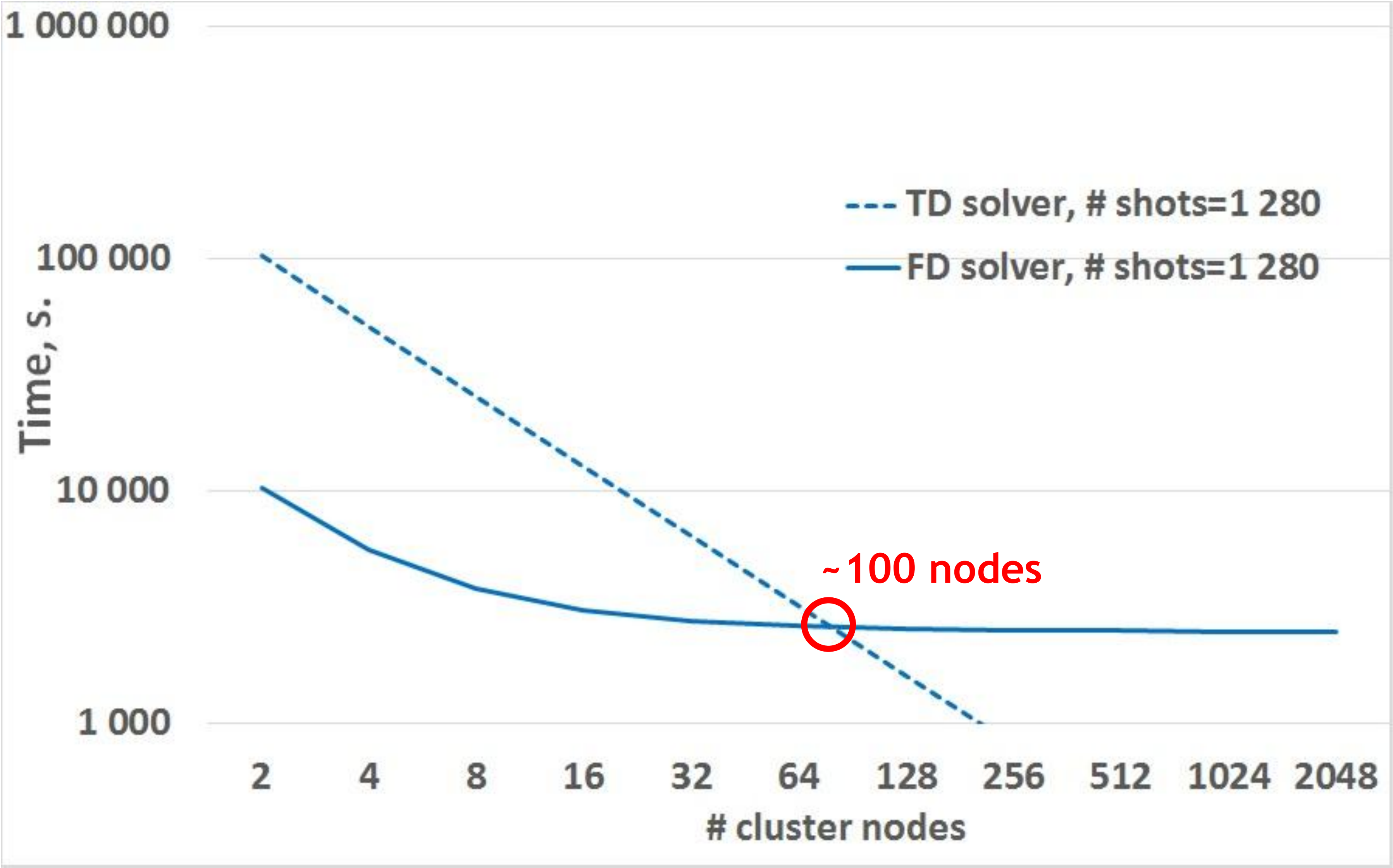


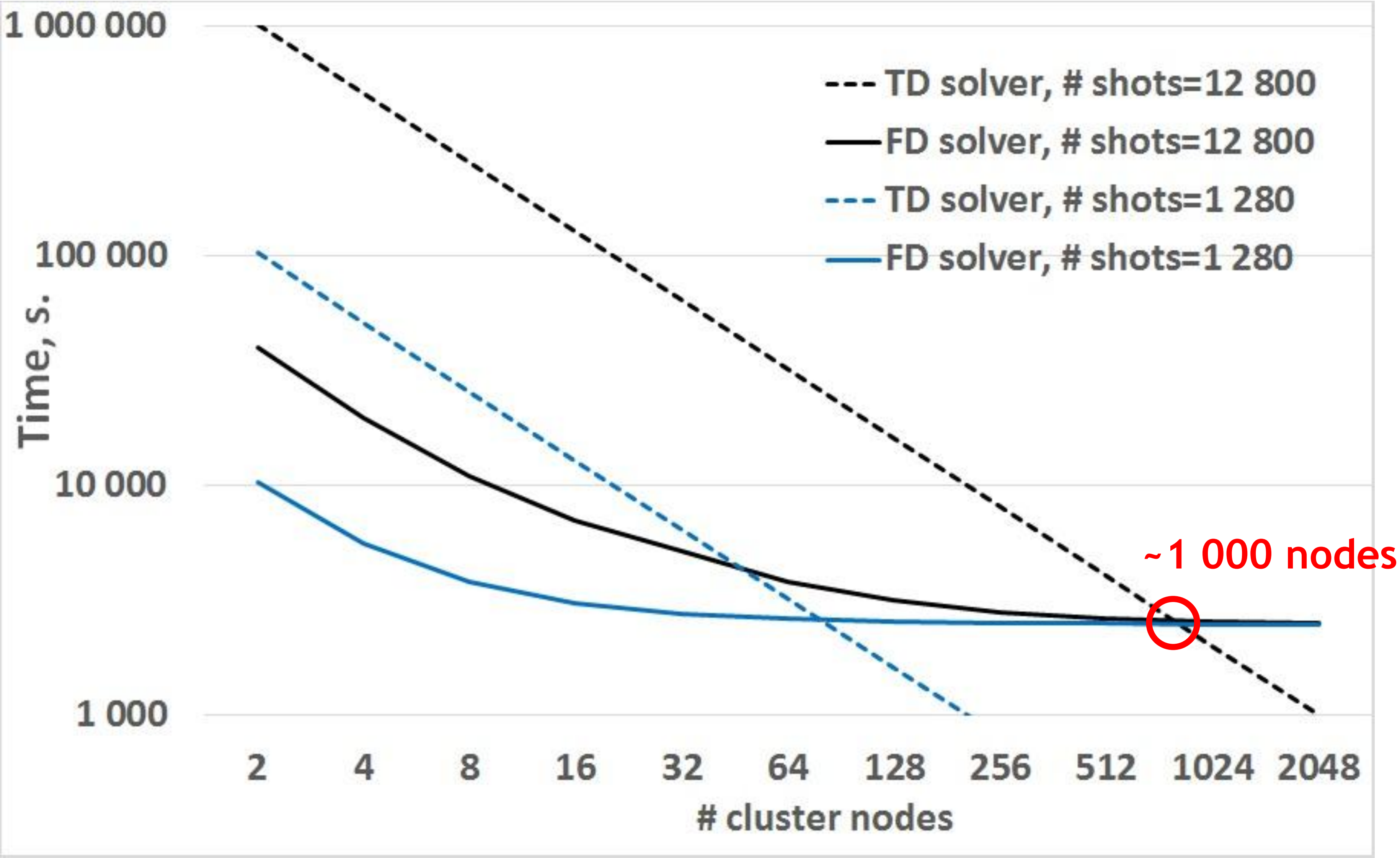
# Timing results: Frequency Domain solver scalability



# Timing results: Time vs. Frequency Domain solvers



# Timing results: Time vs. Frequency Domain solvers





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# Timing results: Time vs. Frequency Domain solvers

**Time Domain**

✓ Ideal scalability => Small computational time for many nodes

$$T_{TD}(N_{proc}, N_{shots}) = T_{TD}(1,1)\max(\frac{N_{shots}}{N_{proc}}, 1)$$

**Frequency domain (HSS)**

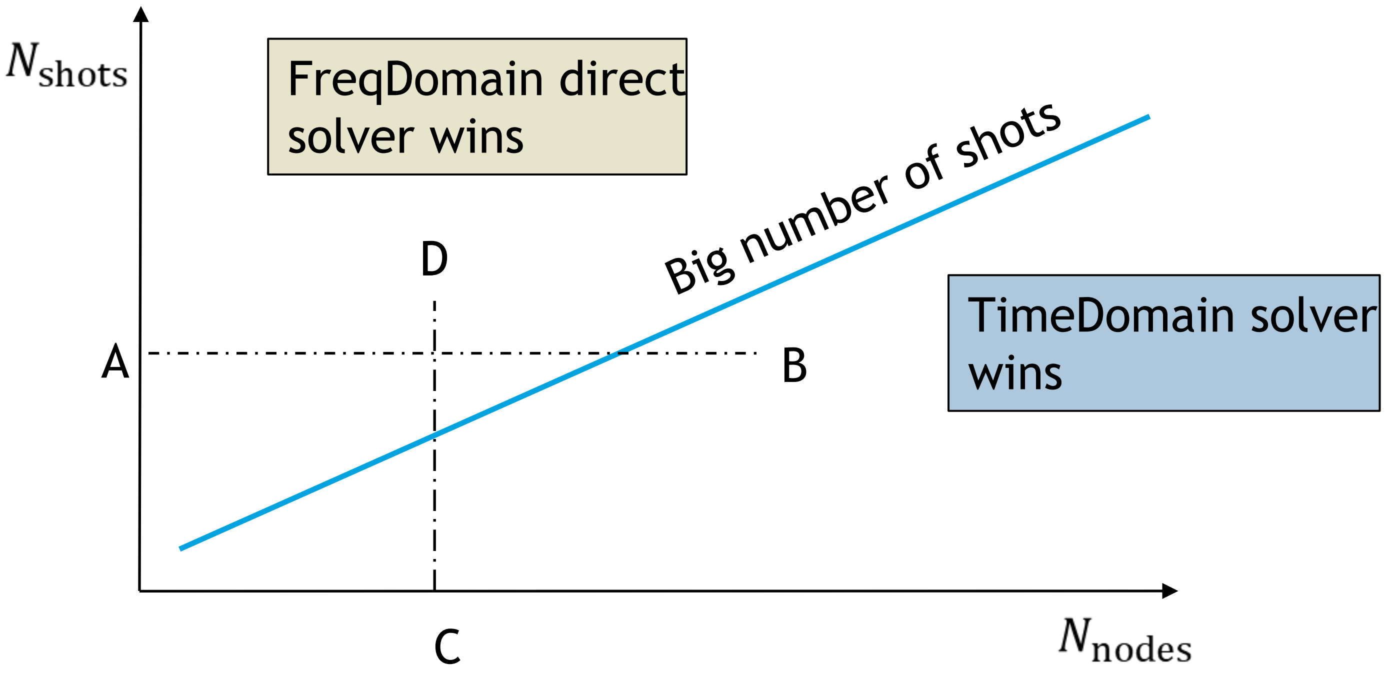
✓ Small computational time for many shots and fixed nodes

$$T_{FD}(N_{proc}, N_{shots}) = T_{FCT}(N_{proc}) + T_{SLV}(N_{proc}, 1)N_{shots}$$

| $\frac{t_{TD},(s)}{t_{HSS},(s)}$ | | $N_{shots}$: 1 | 128 | 1 280 | 12 800 |
|---|---|---|---|---|---|
| $N_{nodes}$ | 32 | 161 / 2 945 | 644 / 2 978 | 6 440 / 3 275 | 64 400 / 6 245 |
| | 64 | 161 / 2 625 | 322 / 2 648 | 3 220 / 2 857 | 32 200 / 4 945 |
| | 128 | 161 / 2 555 | 161 / 2 575 | 1 610 / 2 757 | 16 100 / 4 570 |

Table. Ratios with $t_{TD}$ in the numerator and $t_{HSS}$ in the denominator (BLUE – the HSS is faster).

# Relative performance: Time vs. Frequency Domain solvers




- The blue line defines the "line of equal performance" of the two solvers. For a given number of nodes ($N_{\text{nodes}}$), this line defines the number of shots that is "big enough" to fully reap the benefits of the HSS solver and reach the numerical performance of TDFD.

# Acknowledgments

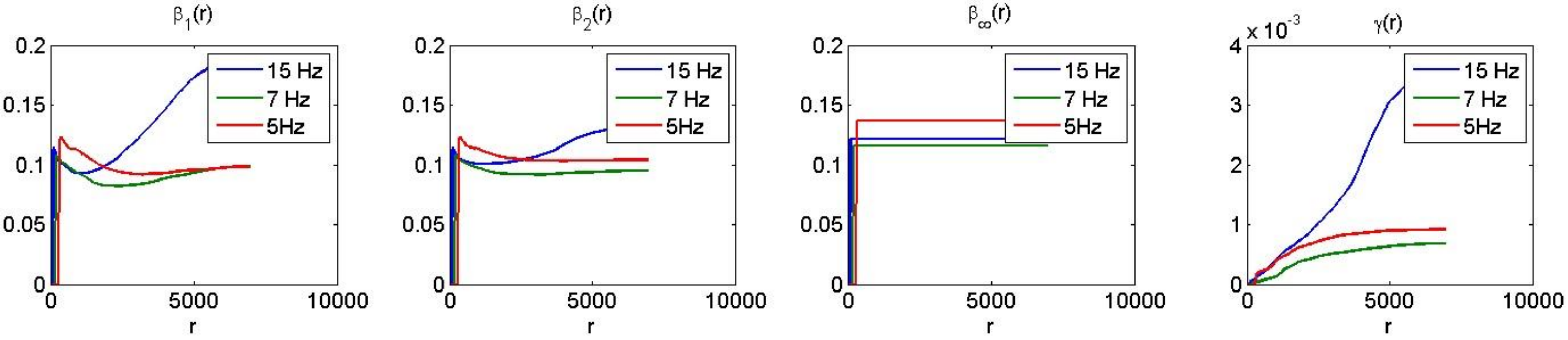
The authors are grateful to:

- GPT EXPEC ARC team for valuable comments and discussions
- KAUST for providing access to cluster Shaheen II

# Q&A

# BACKUP

# Difference between solutions obtained with TD and HSS solvers




Functions $\beta_k(r), \gamma(r)$ are computations of the norms $\beta_k(u,v) = \frac{\|u-v\|_k}{\|u\|_k}$, $k = 1,2$ and $\gamma(u,v) = \left|1 - \left|\frac{(u,v)}{\|u\|\|v\|}\right|\right|$ for balls of radius $r$ (exclude a ball of small radius $r_0$) and centered at the source point; $u = p_{\mathrm{HSS}}, v = p_{\mathrm{TDFD}}$ .