Large-scale Ultrasound Simulations with Local Fourier Basis Decomposition

Jiri Jaros[1], Matej Dohnal[1], Bradley E. Treeby[2]

[1]Faculty of Information Technology, Brno University of Technology, CZ
[2]Department of Medical Physics and Bioengineering, University College London, UK

k-Wave
A MATLAB toolbox for the time-domain simulation of acoustic wave fields

1 Overview

High-intensity focused ultrasound (HIFU) is an emerging non-invasive cancer therapy that uses tightly focused ultrasound waves to destroy tissue cells through localised heating. The treatment planning goal is to select the best transducer position and transmit parameters to accurately target the tumour. The path of the ultrasound waves can be predicted by solving acoustic equations based on mass, momentum, and energy conservation. However, this is a computationally difficult problem because the domain size is very large compared to the acoustic wavelength.
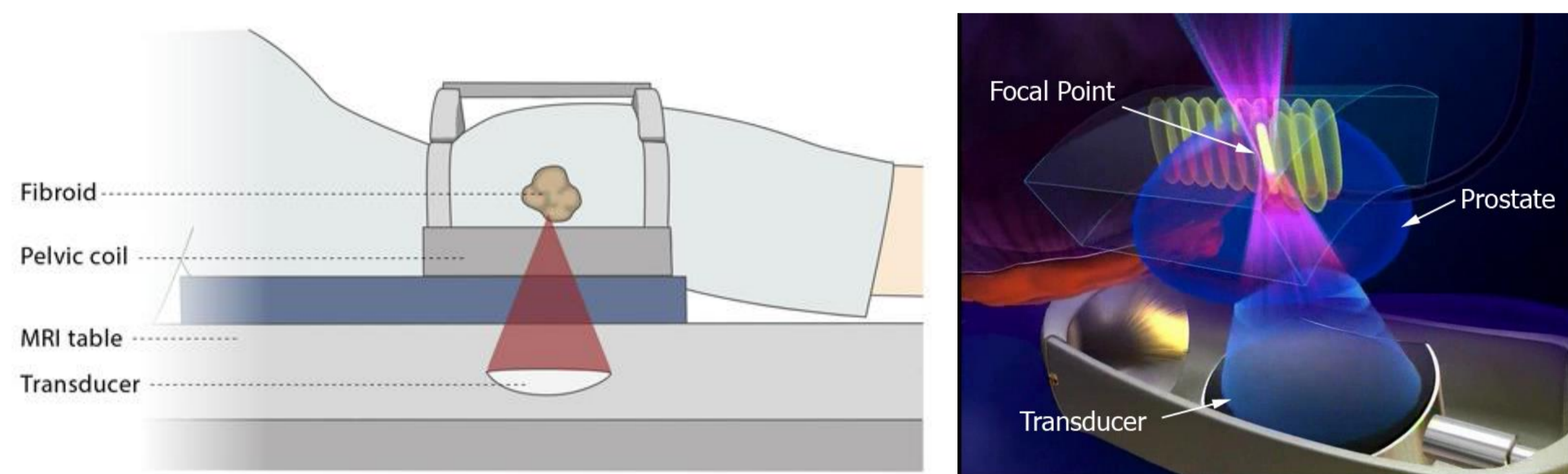
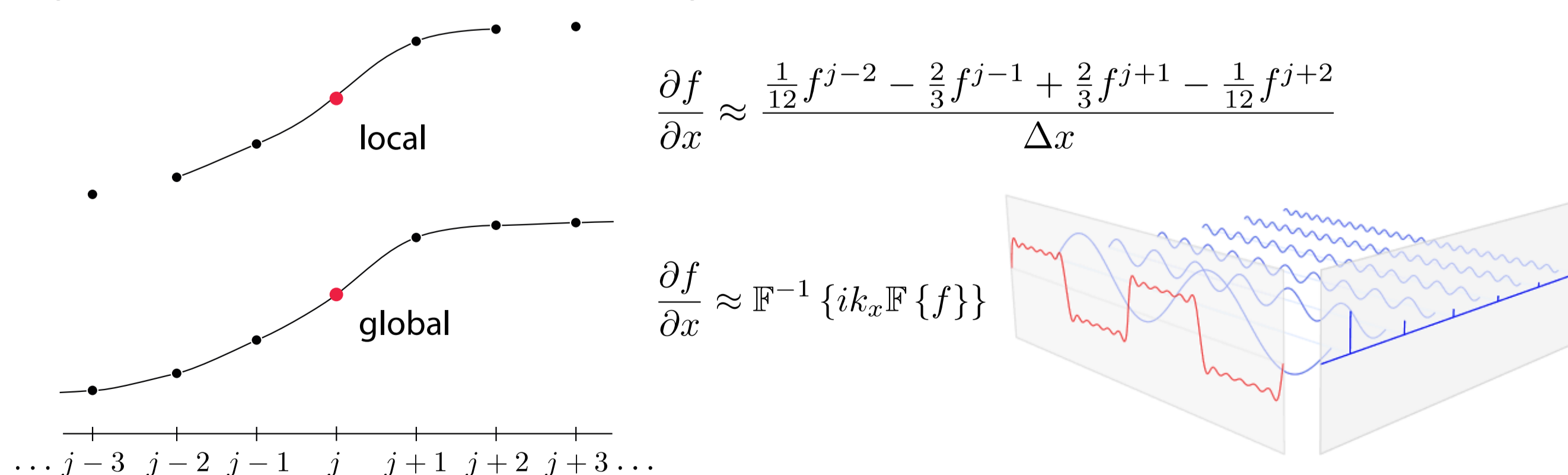## 2 Nonlinear Ultrasound Wave Propagation in Tissue

The governing equations must account for the nonlinear propagation of ultrasound waves in tissue, which is a heterogeneous and absorbing medium. Accurately accounting for acoustic absorption is critical for predicting ultrasound dose under different conditions. The required acoustic equations can be written as:

$$\frac{\partial \mathbf{u}}{\partial t} = -\frac{1}{\rho_0}\nabla p \qquad \text{momentum conservation}$$

$$\frac{\partial \rho}{\partial t} = -(2\rho + \rho_0)\nabla \cdot \mathbf{u} - \mathbf{u} \cdot \nabla \rho_0 \qquad \text{mass conservation}$$

$$p = c_0^2 \left(\rho + \mathbf{d} \cdot \nabla \rho_0 + \frac{B}{2A}\frac{\rho^2}{\rho_0} - \Pi\rho \right) \qquad \text{pressure-density relation}$$

These equations are discretised using the *k-space* pseudo-spectral method and solved iteratively. This reduces the number of required grid points per wavelength by an order of magnitude compared to finite element or finite difference methods. For uniform Cartesian grids, the gradients can be calculated using the fast Fourier transform (FFT).

$$\frac{\partial f}{\partial x} \approx \frac{\frac{1}{12}f^{j-2} - \frac{2}{3}f^{j-1} + \frac{2}{3}f^{j+1} - \frac{1}{12}f^{j+2}}{\Delta x}$$

$$\frac{\partial f}{\partial x} \approx \mathbb{F}^{-1}\{ik_x\mathbb{F}\{f\}\}$$

$\dots j-3 \quad j-2 \quad j-1 \quad j \quad j+1 \quad j+2 \quad j+3 \dots$

3 Global Domain Decomposition

The 1D global domain decomposition is the natural way of partitioning simulation domains while using spectral methods. This decomposition offers great accuracy, however, it suffers from all-to-all communication bottleneck and limited scaling given by the longest domain size.
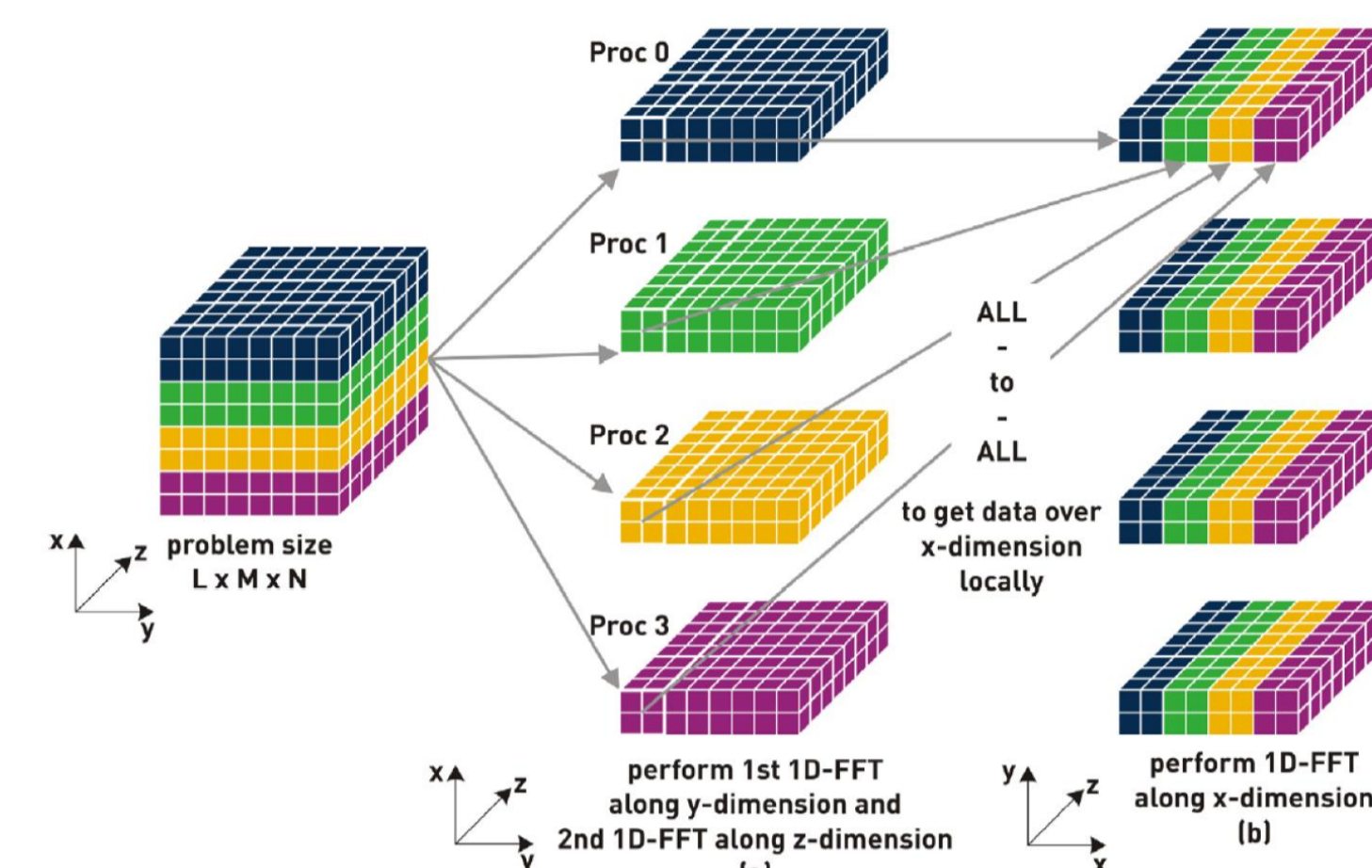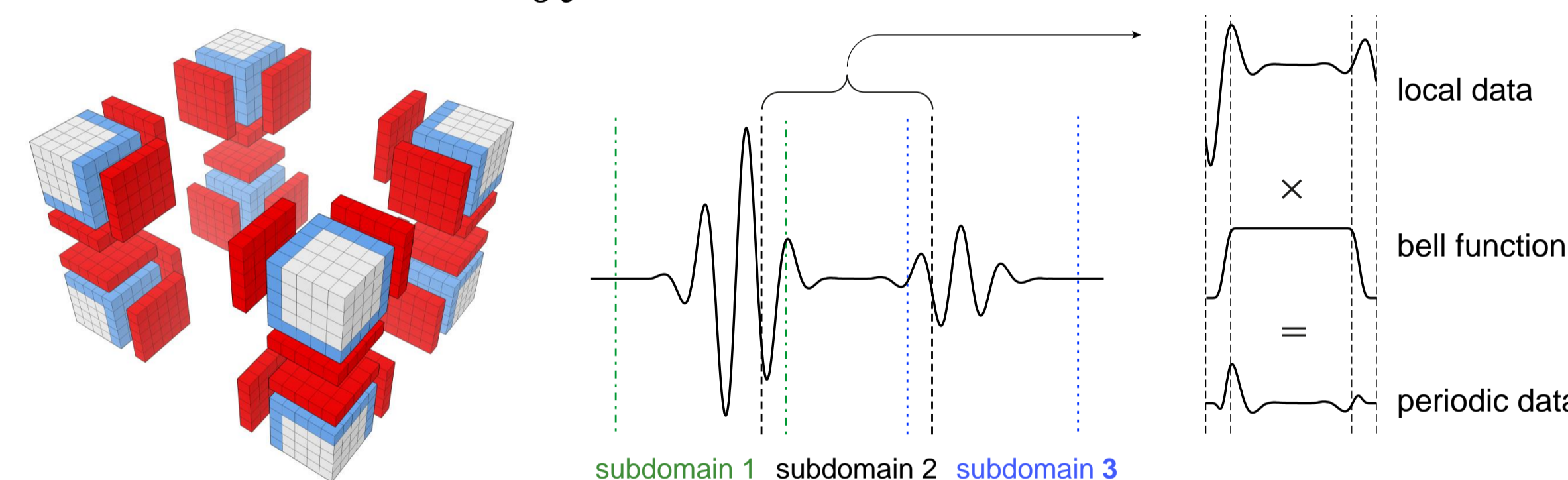

4 Local Fourier Basis Decomposition

Local domain decomposition reduces the communication burden by partitioning the domain into a grid of local subdomains where gradients are calculated locally and the global communication is replaced by the nearest-neighbor halo exchange.

The gradient calculation with the hallo on an *i*-th subdomain reads as follows (*b* is a bell function smoothening the subdomain interface):

$$\frac{\partial p_i}{\partial t} = \mathbb{F}^{-1}\{ik_i\mathbb{F}(b \cdot p_i)\}$$

local data
bell function
periodic data

subdomain 1   subdomain 2   subdomain 3
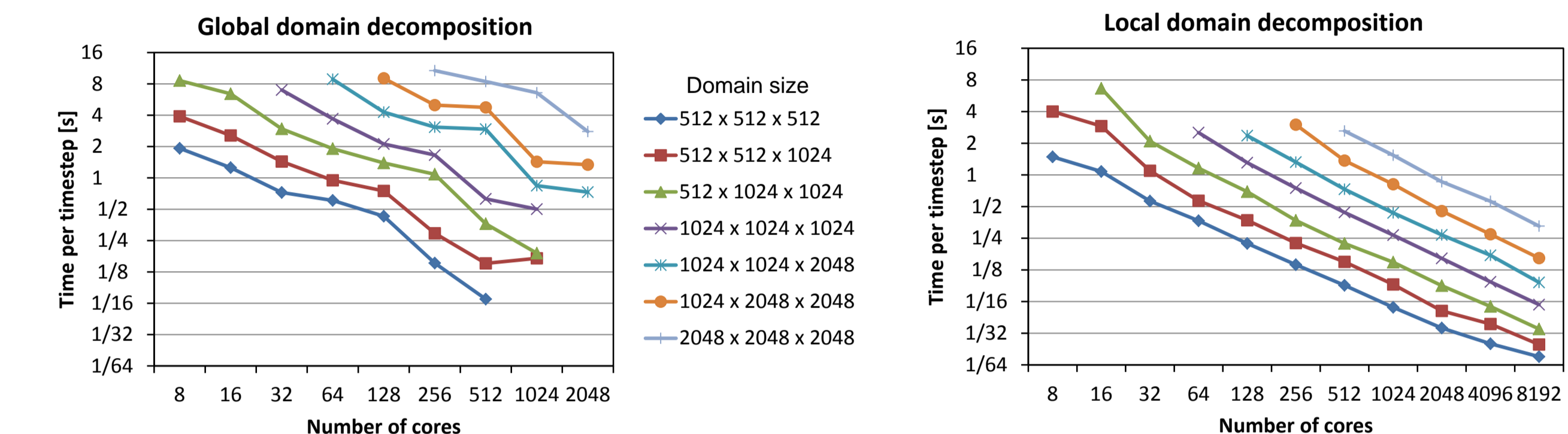
5 Local Decomposition Accuracy

Since the gradient is not calculated on the whole data, numeric error is introduced. Its level can be tuned by the thickness of the halo region and the shape of the bell function.

An appropriate thickness of 16 grid points and the bell shape were experimentally set as a tradeoff between accuracy and performance.
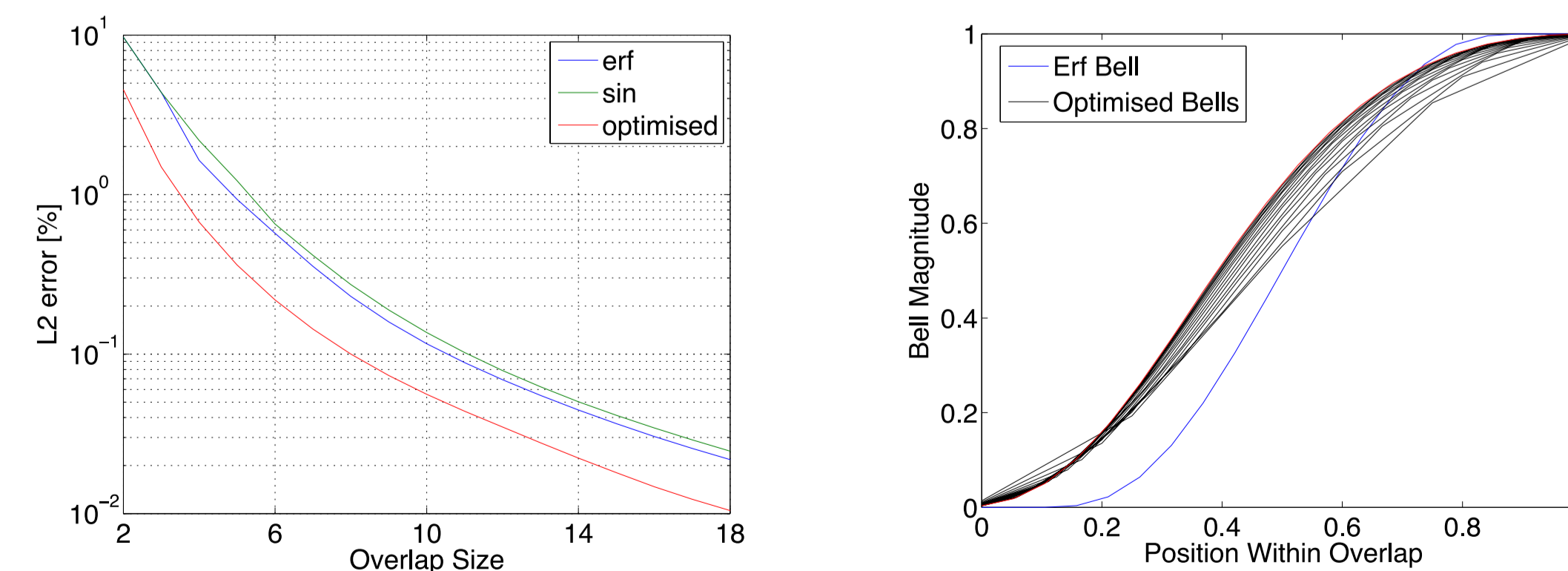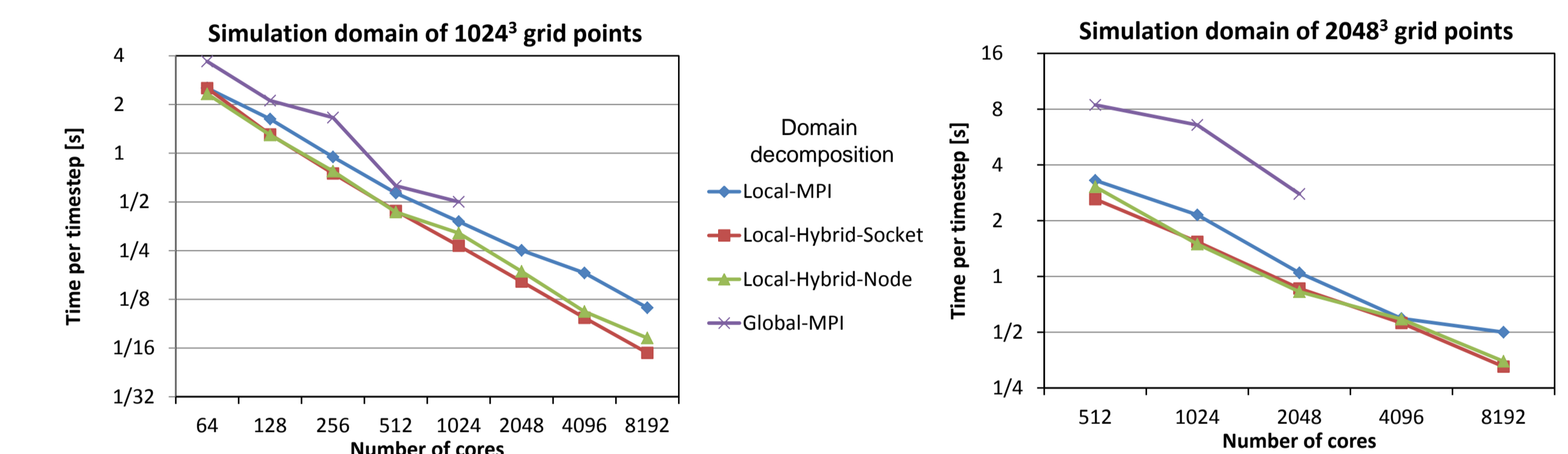

6 Strong Scaling Comparison

Significant improvements in the strong scaling were achieved on the whole simulation size range <512³, 2048³> grid points while using 8 to 8192 cores of SuperMUC. All the scaling curves go longer, steeper and smoother.

Global domain decomposition

Local domain decomposition

Domain size
512 x 512 x 512
512 x 512 x 1024
512 x 1024 x 1024
1024 x 1024 x 1024
1024 x 1024 x 2048
1024 x 2048 x 2048
2048 x 2048 x 2048

The local Fourier basis decomposition was implemented using both pure-MPI and hybrid OpenMP/MPI paradigms. The benefits mainly show up for large domains offering up to 8.55 times higher performance compared to the global decomposition.

Simulation domain of 1024³ grid points

Simulation domain of 2048³ grid points

Domain decomposition
Local-MPI
Local-Hybrid-Socket
Local-Hybrid-Node
Global-MPI

7 Result of Ultrasound Simulation

An example of a realistic HIFU kidney treatment simulation output (distribution of the maximum acoustic pressure).

Transverse plane

Sagittal plane

focal distortion
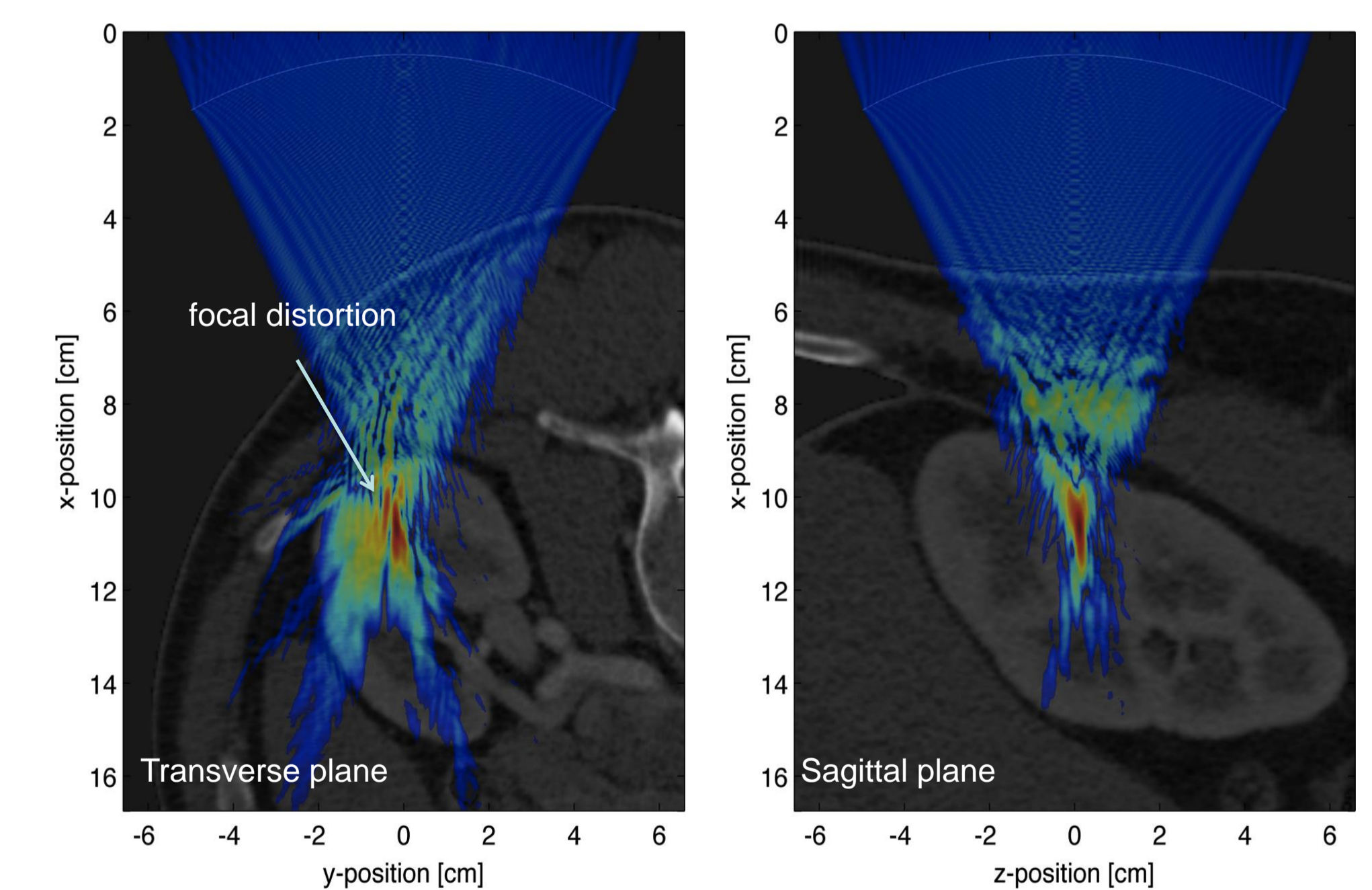
Simulation size 2048x1536x1536 grid points, 170x135x135mm. Max ultrasound frequency 8MHz, 500W/cm² focal intensity. Calculated in 40.5 hours on 768 cores with 760 GB of RAM.