Scalable Direct Solver for Compact Stencil Calculation on Rectangular Grid

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3D Helmholtz Equation

The model problem considered is the numerical solution of

$$\nabla^2 u + k^2 u = f, \quad \text{in } \Omega, \tag{1}$$

where k is a complex valued coefficient depending only on z. The Dirichlet boundary condition is considered.

Detecting Subsurface Objects

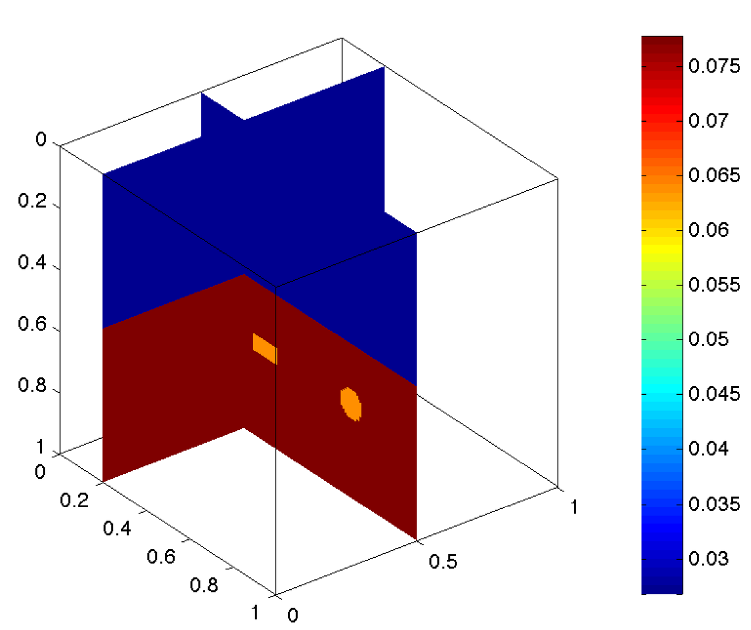


Figure 1: Subsurface objects

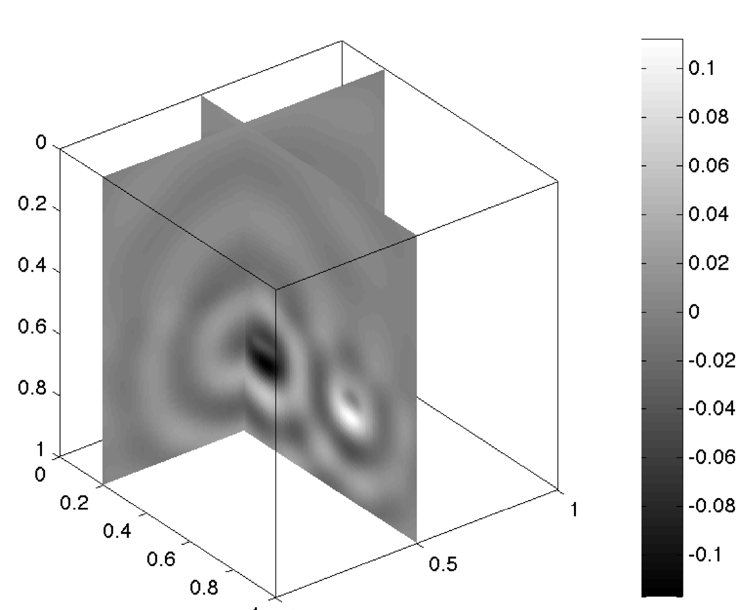


Figure 2: Scattered waves

High Resolution Compact Schemes

Each of the schemes for the approximation of the solution to (1) can be written as

$$L^{(n)} u = F^{(n)} \tag{2}$$

where $L^{(n)}$, $n = 2, 4, 6$ is an n^{th} order approximation finite-difference operator and $F^{(n)}$ is the corresponding right hand side.

$$L^{(2)} = h_z^2 \left(\delta_{xx} + \delta_{yy} + \delta_{zz} + k^2 I\right)$$

$$L^{(4)} = h_z^2 \Big[\delta_{xx} + \delta_{yy} + \delta_{zz} + \frac{1}{6}(h_x^2 + h_y^2)\delta_{xx}\delta_{yy}$$

$$+ \frac{1}{6}(h_x^2 + h_z^2)\delta_{xx}\delta_{zz} + \frac{1}{6}(h_y^2 + h_z^2)\delta_{yy}\delta_{zz}$$

$$+ k^2 \left[I + \frac{h_x^2}{12}\delta_{xx}^2 + \frac{h_y^2}{12}\delta_y^2 + \frac{h_z^2}{12}\delta_{zz}^2\right]\Big]$$

(Lele, 1992)

$$L^{(6)} = h^2(\delta_{xx} + \delta_{yy} + \delta_{zz})\left(1 + \frac{k^2 h^2}{30}\right) u + k^2 h^2 u$$

$$+ \frac{h^4}{6}(\delta_{xx}\delta_{yy} + \delta_{xx}\delta_{zz} + \delta_{yy}\delta_{zz})\left(1 + \frac{k^2 h^2}{15}\right) u$$

$$+ \frac{h^6}{30}\delta_{xx}\delta_{yy}\delta_{zz} u + \frac{h^4}{20}\left((k^2)_{zz} - k^4\right) u$$

$$+ \frac{h^3}{10}(k^2)_z \left[h\delta_z u + \frac{h^3}{6}\left[\delta_{xxz} u + \delta_{yyz} u + \delta_z (k^2 u)\right]\right]$$

(E. Turkel, D. and R. Gordon, S. Tsynkov, 2014)

Generalized 27-Point Stencil

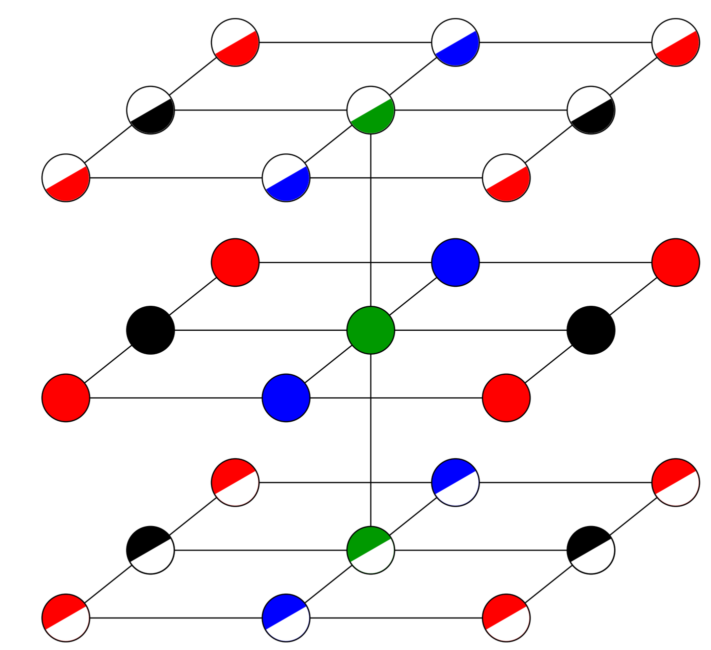


Figure 3: Systems with the same stencil can be solved with this algorithm.

FFT Type Direct Solver

The system (2) can be presented in the form

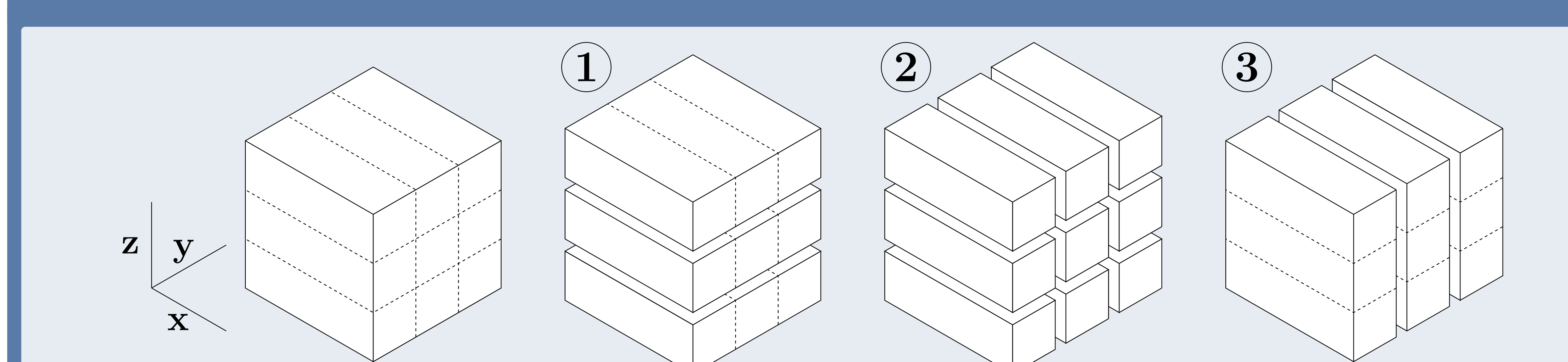
$$C_1 U_{l-1} + C_2 U_l + C_3 U_{l+1} = F_l$$

for $l = 1 \ldots N_z$, where C_1, C_2 and C_3 are $N_x \cdot N_y \times N_x \cdot N_y$ matrices. Let V be a matrix consisting of the set of orthonormal eigenvectors of C_1, C_2 and C_3. Hence the matrices $\Lambda_1 = V^T C_1 V$, $\Lambda_2 = V^T C_2 V$ and $\Lambda_2 = V^T C_2 V$ are the diagonal matrices of eigenvalues. It follows

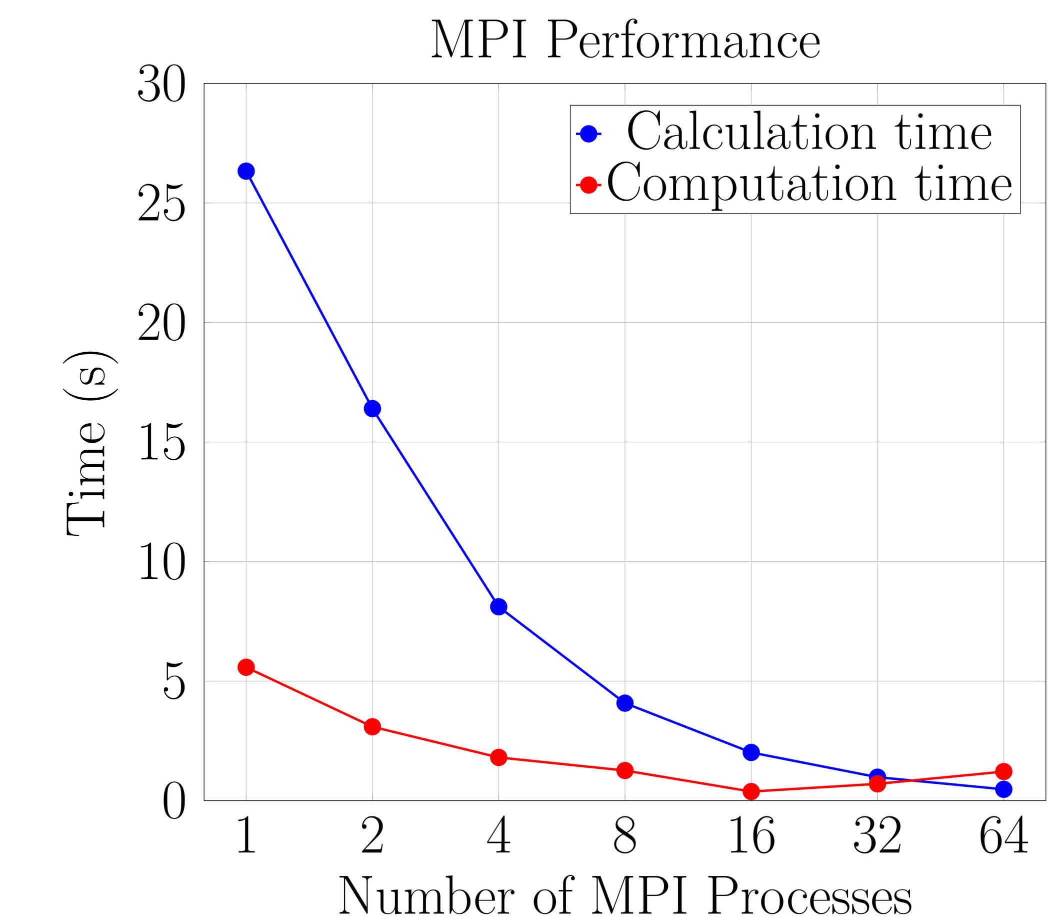
$$C_1 U_{l-1} + C_2 U_l + C_3 U_{l+1} = F_l$$
$$\Lambda_1 W_{l-1} + \Lambda_2 W_l + \Lambda_3 W_{l+1} = \bar{F}_l$$

where $W_l = V^T U_l$, $\bar{F}_l = V^T F_l$ and the transformed right hand side, $\bar{F}_l$, can be obtained from F_l by the discrete sine transform (DST) via parallel FFT. This direct solution requires $O(N_x N_y N_z \log N)$ operations, where $N = \max(N_x, N_y)$.

MPI Data Transfer



Results



Grid	Nodes	Processors	Time (s)
512^3	1	32	2.830525
1024^3	4	128	8.759851
2048^3	32	1024	40.465395
4096^3	256	4096	445.803343

Table 1: MPI

Grid	Nodes	Processors	Time (s)
512^3	1	32	7.793963
1024^3	4	128	16.911352
2048^3	32	1024	19.417831
4096^3	256	8192	27.522366

Table 2: Hybrid

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