FFT-based homogenisation accelerated by low-rank approximations

Jaroslav Vondřejc [1], Dishi Liu [1], **Martin Ladecký [2]** and Hermann G. Matthies[1]

[1]Institute of Scientific Computing, Technische Universität Braunschweig

[2]Department of Mathematics, Faculty of Civil Engineering,
Czech Technical University in Prague

AANMPDE 12, Strobl, Austria

software FFTHomPy Preprint martin.ladecky@fsv.cvut.cz

Outline

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- Analysis of heterogeneous (composite) materials (HeM).
- Homogeneously describe HeM constitutive behavior.
- Materials with periodic microstructure.

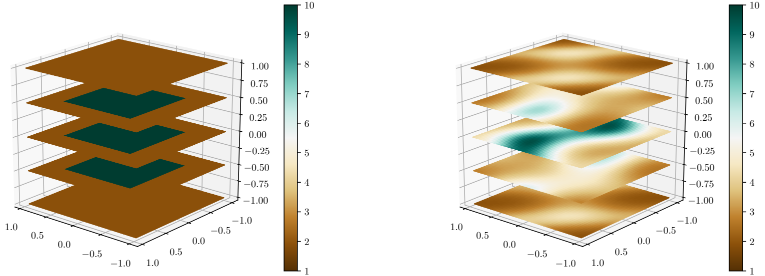

Figure 1: Representative volume elements of periodic heterogeneous microstructure in 3D.

A model problem in homogenization

- Input: Heterogeneous material property

$$\boldsymbol{A}(\boldsymbol{x}) : \mathcal{Y} \to \mathbb{R}^{d\times d} \quad \text{in} \quad \mathcal{Y} = \left(-\frac{1}{2}, \frac{1}{2}\right)^d, \quad d = 2, 3.$$

- Output: Homogenized (constant) material property

$$\boldsymbol{A}_{\mathrm{H}} \in \mathbb{R}^{d\times d}$$

- Integral over domain

$$\boldsymbol{A}_{\mathrm{H}} \boldsymbol{E}_\alpha = \frac{1}{|\mathcal{Y}|} \int_{\mathcal{Y}} \boldsymbol{A}(\boldsymbol{x})(\boldsymbol{E}_\alpha + \nabla u_\alpha)\,\mathrm{d}\boldsymbol{x}, \quad \alpha = 1, \ldots, d.$$

- Elliptic PDE with periodic b.c. on rectangular domain

$$\nabla \cdot (\boldsymbol{A}(\boldsymbol{x}) \nabla u_\alpha) = -\nabla \cdot \boldsymbol{A}(\boldsymbol{x}) \boldsymbol{E}_\alpha \quad \text{in} \quad \mathcal{Y}, \quad \alpha = 1, \ldots, d.$$

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Fourier-Galerkin method

- Elliptic PDE with periodic boundary conditions

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- A uniform grid discretization $\boldsymbol{N} = [N_1, \dots, N_d] \in \mathbb{R}^d$.
- Approximation with trigonometric polynomials[1],

$$u(\boldsymbol{x}) \approx \sum_{\boldsymbol{k}\in\mathbb{Z}_{\boldsymbol{N}}} \mathrm{u}(\boldsymbol{x}_{\boldsymbol{N}}^{\boldsymbol{k}})\varphi_{\boldsymbol{N}}^{\boldsymbol{k}}(\boldsymbol{x}) = \sum_{\boldsymbol{k}\in\mathbb{Z}_{\boldsymbol{N}}} \widehat{\mathrm{u}}[\boldsymbol{k}]\varphi^{\boldsymbol{k}}(\boldsymbol{x}),$$

where $\varphi^{\boldsymbol{k}}(\boldsymbol{x}) = \exp(2\pi \mathrm{i}\boldsymbol{k} \cdot \boldsymbol{x})$ and

$$\mathcal{F}_{\boldsymbol{N}}\mathbf{u} = \widehat{\mathbf{u}}$$

where $\mathcal{F}_{\boldsymbol{N}}$ is Fourier transform.

[1] Jan Zeman, Jaroslav Vondřejc, Jan Novák, Ivo Marek, 2010, Accelerating a FFT-based solver for numerical homogenization of periodic media by conjugate gradients.

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- Applied in Fourier space:
- The gradient: $\widehat{\nabla}_{\boldsymbol{N}} : \mathbb{C}^{\boldsymbol{N}} \to \mathbb{C}^{d\times\boldsymbol{N}}$

$$\nabla u(\boldsymbol{x}) = \sum_{\boldsymbol{k}\in\mathbb{Z}_{\boldsymbol{N}}} \widehat{\mathrm{u}}[\boldsymbol{k}]\nabla\varphi^{\boldsymbol{k}}(\boldsymbol{x}) = \sum_{\boldsymbol{k}\in\mathbb{Z}_{\boldsymbol{N}}} 2\pi\mathrm{i}\boldsymbol{k}\widehat{\mathrm{u}}[\boldsymbol{k}]\varphi^{\boldsymbol{k}}(\boldsymbol{x}),$$

which corresponds to $(\widehat{\nabla}_{\boldsymbol{N}}\widehat{\mathbf{u}})[\alpha,\boldsymbol{k}] = 2\pi\mathrm{i}k_\alpha\widehat{\mathbf{u}}[\boldsymbol{k}]$.

- The divergence: $\widehat{\nabla}^*_{\boldsymbol{N}} : \mathbb{C}^{d\times\boldsymbol{N}} \to \mathbb{C}^{\boldsymbol{N}}$

$$(\widehat{\nabla}^*_{\boldsymbol{N}}\widehat{\mathbf{w}})[\boldsymbol{k}] = \sum_{\alpha=1}^{d} 2\pi\mathrm{i}k_\alpha\widehat{\mathbf{w}}[\alpha,\boldsymbol{k}].$$

- PDE

$$\nabla \cdot (\boldsymbol{A}(\boldsymbol{x}) \nabla u) = -\nabla \cdot \boldsymbol{A}(\boldsymbol{x}) \boldsymbol{E} \quad \text{in} \quad \mathcal{Y}.$$

- The linear system

$$\underbrace{\mathcal{F}_{\boldsymbol{N}}^{-1} \widehat{\nabla}_{\boldsymbol{N}}^{*} \mathcal{F}_{\boldsymbol{N}} \widetilde{\mathbf{A}} \mathcal{F}_{\boldsymbol{N}}^{-1} \widehat{\nabla}_{\boldsymbol{N}} \mathcal{F}_{\boldsymbol{N}}}_{\mathbf{C}} \mathbf{u} = \underbrace{-\mathcal{F}_{\boldsymbol{N}}^{-1} \widehat{\nabla}_{\boldsymbol{N}}^{*} \mathcal{F}_{\boldsymbol{N}} \widetilde{\mathbf{A}} \mathbf{E}}_{\mathbf{d}}, \quad \mathbf{u} \in \mathbb{R}^{N_1 \times \cdots \times N_d}.$$

  - The system $\mathbf{Cu} = \mathbf{d}$, solved with Richardson iteration

$$\mathbf{u}_{(i+1)} = [\mathbf{u}_{(i)} + \omega(\mathbf{d} - \mathbf{C}\mathbf{u}_{(i)})].$$

Linear system

- PDE

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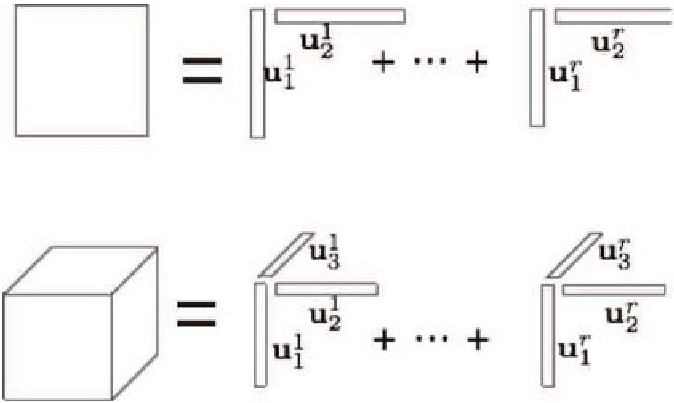
Outline

Idea of low-rank tensor approximation



[2]

Figure 2: Low-rank decomposition of a second-order tensor (matrix) (top), and a third-order tensor (bottom).

[2] Zhang, Zheng and Batselier, Kim and Liu, Haotian and Daniel, Luca and Wong, Ngai, *Tensor Computation: A New Framework for High-Dimensional Problems in EDA*, IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems

Idea of low-rank tensor approximation

- In 2D we can express tensor(matrix) $\mathbf{v} \in \mathbb{C}^{N \times N}$ in the form

$$\mathbf{v} = \sum_{i=1}^{N} c[i] \mathbf{b}_i^{(1)} \otimes \mathbf{b}_i^{(2)},$$

  where $\mathbf{b}_i^{\alpha} \in \mathbb{C}^N$ is i-th basis vectors in spatial direction α.

- Strongly decreasing sequence of coefficients c[i].
- Approximation with r "significant" vectors

$$\mathbf{v} \approx \widetilde{\mathbf{v}} = \sum_{i=1}^{r} c[i] \mathbf{b}_i^{(1)} \otimes \mathbf{b}_i^{(2)}.$$

- Memory requirement of full format is N^d and low-rank is dNr.

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Canonical format[3]

- The representation has the form:

$$\mathbf{v} \approx \sum_{i=1}^{r} \bigotimes_{j=1}^{d} \mathbf{b}_{\mathbf{v}}^{(j)}[i_j].$$

  where item $\mathbf{b}_{\mathbf{v}}^{(j)} \in \mathbb{C}^{r \times N_j}$ stores the basis vectors.

- obtained by Singular Value Decomposition (SVD).
- Memory requirements: dNr
- Pros: The lowest memory requirements.
- Cons: only in 2D.

[3] Hackbusch,Wolfgang: Tensor Spaces and Numerical Tensor Calculus, Springer Verlag Berlin Heidelberg New York, 2012.

Tucker format[4]

- Generalisation of the canonical format to higher dimensions.
- The representation has the form:

$$\mathbf{v} \approx \sum_{i_1=1}^{r_1} \cdots \sum_{i_d=1}^{r_d} \mathrm{c}[i_1, \ldots, i_d] \bigotimes_{j=1}^{d} \mathbf{b}_{\mathbf{v}}^{(j)}[i_j].$$

  where $\mathrm{c}[i_1, \ldots, i_d]$ is element of core $\mathbf{c} \in \mathbb{C}^{r_1 \times \cdots \times r_d}$.
- obtained by Higher Order Singular Value Decomposition (HOSVD).
- Memory requirements: $dNr + r^d$.
- Pros: higher dimensions.
- Cons: core size depends exponentially on dimension.

[4] Hackbusch,Wolfgang: Tensor Spaces and Numerical Tensor Calculus, Springer Verlag Berlin Heidelberg New York, 2012.

Tensor train (TT) format[5]

- The representation has the form:

$$\mathbf{v} \approx \sum_{i_1=1}^{r_1} \cdots \sum_{i_{d-1}=1}^{r_{d-1}} \bigotimes_{j=1}^{d} \mathbf{b}_{\mathbf{v}}^{j}[i_{j-1}, :, i_j],$$

  where $\mathbf{b}_{\mathbf{v}}^{j} \in \mathbb{C}^{r_{j-1} \times N_j \times r_j}$ are the *carriages*.

- Memory requirements: $2Nr + (d-2)Nr^2$
- Pros: size depends linearly on d.
- Cons: Truncation is more expensive.

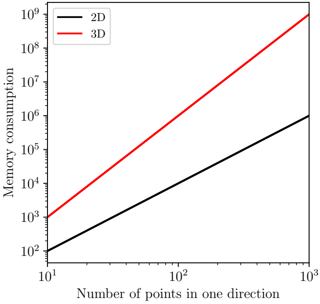
[5]Oseledets, Ivan and Tyrtyshnikov, Eugene: Linear Algebra Appl.,North-Holland, TT-cross approximation for multidimensional arrays, 2010, pp 0–88.

Linear system with low-rank tensors

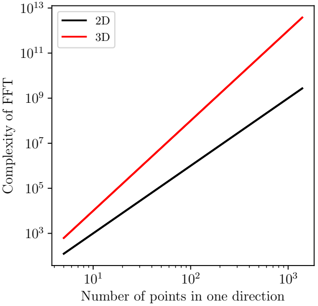
- The linear system

$$\underbrace{\mathcal{F}_{\boldsymbol{N}}^{-1}\widehat{\nabla}^{*}_{\boldsymbol{N}}\mathcal{F}_{\boldsymbol{N}}\widetilde{\mathbf{A}}\mathcal{F}_{\boldsymbol{N}}^{-1}\widehat{\nabla}_{\boldsymbol{N}}\mathcal{F}_{\boldsymbol{N}}}_{\mathbf{C}}\mathbf{u} = \underbrace{-\mathcal{F}_{\boldsymbol{N}}^{-1}\widehat{\nabla}^{*}_{\boldsymbol{N}}\mathcal{F}_{\boldsymbol{N}}\widetilde{\mathbf{A}}\mathbf{E}}_{\mathbf{d}},$$

- Memory consumption of **u**



- Complexity of FFT



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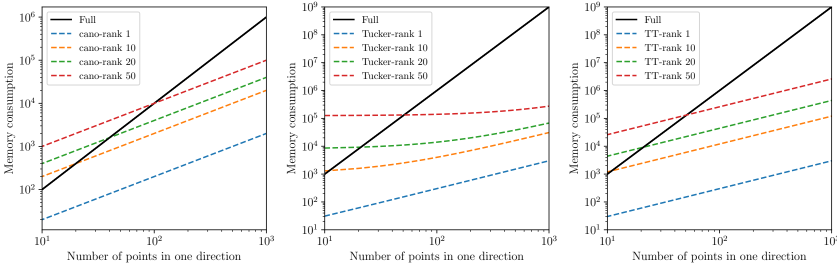

Figure 3: Memory consumption of canonical in 2D (left), Tucker (middle) and TT (right) in 3D.

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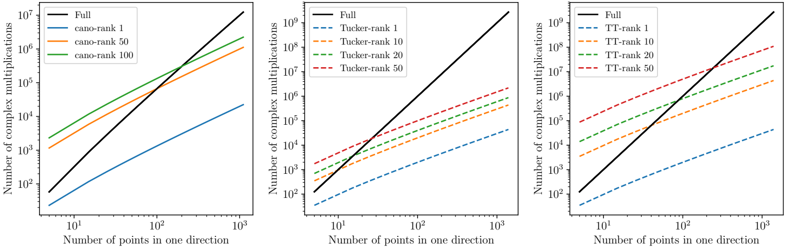

FIGURE 4: FFT complexity of canonical in 2D (left), Tucker (middle) and TT (right) in 3D.

- Mathematical operations are performed in low rank format.
- Rank grows during some operations (see Table 1).

Operation	Rank r
Differentiation (gradient)	remain unchanged
d-dimensional FFT	remain unchanged
Evaluation of material law	increased
Divergence	increased

TABLE 1: Effect of operations in low-rank formats on rank r.

- Rank truncation (rounding) $\mathcal{T}$ - keep rank on efficient level.
  - require additional operations

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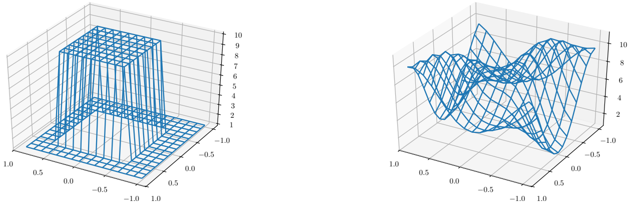
Outline

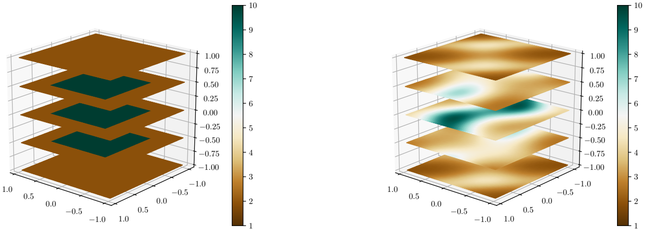
1. Introduction to FFT-based Homogenisation
   - Homogenisation problem
   - Fourier-Galerkin method
2. Low-Rank Tensor Approximations
   - Idea of low-rank tensor Approximation
   - Low-rank tensor formats
   - Linear system with low-rank tensors
3. Numerical Experiments and Results
4. Conclusion

Materials

- Canonical in 2D:



- Tucker and TT in 3D:



Error of low-rank approximation

- As an criterion the relative algebraic error between the low-rank solution and the full solution has been used, i.e.

$$\text{relative error} = \frac{A_{\mathrm{H},\boldsymbol{N}} - \tilde{A}_{\mathrm{H},\boldsymbol{N}}}{A_{\mathrm{H},\boldsymbol{N}}}.$$

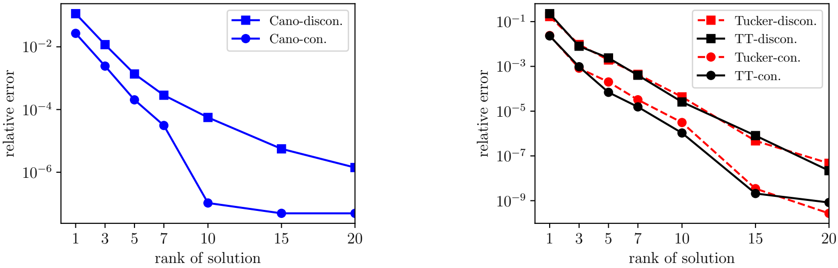


Figure 5: Dependency of approximation error on solution rank.

- memory effectiveness

$$\frac{\text{memory for sparse solution}}{\text{memory for full solution}}$$

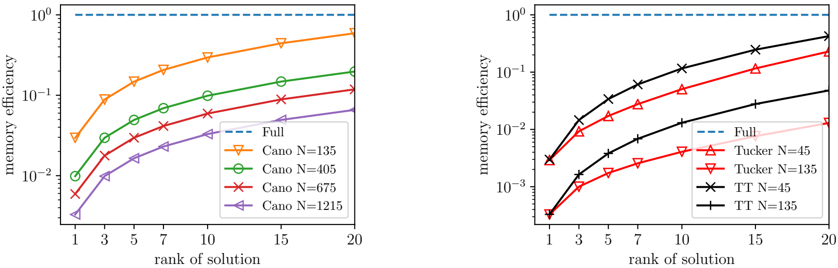
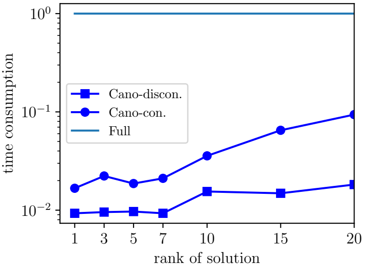


Figure 6: Dependency of memory efficiency on solution rank for discretizations with N^d points.

Computational efficiencies

- Computational effectiveness

$$\frac{\text{time for sparse solution}}{\text{time for full solution}}$$



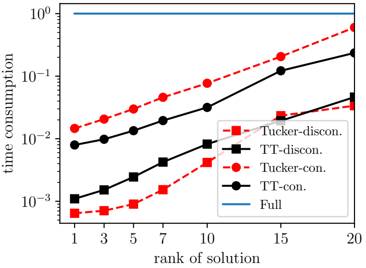


Figure 7: Time consumption with respect to rank-r

Outline

Conclusion

- Elliptic PDE with periodic boundary conditions

$$\nabla \cdot (\boldsymbol{A}(\boldsymbol{x})\nabla u_\alpha) = \nabla \cdot \boldsymbol{A}(\boldsymbol{x})\boldsymbol{E}_\alpha \quad \text{in} \quad \mathcal{Y}, \quad \alpha = 1, \ldots, d.$$

- Solved by FFT-based Fourier-Galerkin method.
- Linear system expressed in low-rank tensor formats.
- Tested formats: canonical, Tucker, and tensor train (TT).
- Low-rank approximations lead to a significant memory and computational reduction.

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Conclusion

- Elliptic PDE with periodic boundary conditions

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Thank you for your attention!

FFT-based homogenisation accelerated by low-rank approximations

Jaroslav Vondřejc [1], Dishi Liu [1], **Martin Ladecký [2]** and Hermann G. Matthies[1]

[1]Institute of Scientific Computing, Technische Universität Braunschweig

[2]Department of Mathematics, Faculty of Civil Engineering,
Czech Technical University in Prague

AANMPDE 12, Strobl, Austria

software FFTHomPy Preprint martin.ladecky@fsv.cvut.cz