SIMPLE-FFT for flow computations in low porosity µCT images

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Summary

In recent years, the oil and gas industries and the soil sciences have begun to embrace the use of µ-CT images of rocks and soils for understanding their material properties. Besides geometric analysis, material properties can also be estimated by post-processing solutions of partial differential equations on the images.

Because such materials with low porosity typically have also low permeability and small pores, it is difficult for gas or liquid to pass through them. For the classical SIMPLE algorithm it is also hard to converge to the solution of the steady state Stokes equations due to the complex connectivity. Solving the pressure correction equation was identified as the bottleneck of convergence. Using the Fast Fourier Transform (FFT) reduces the computation times significantly. The runtime and memory usage of the FFT accelerated SIMPLE method, SIMPLE-FFT, which is integrated in the **GeoDict** software, are compared with Fraunhofer ITWM's in-house Lattice Boltzmann solver, ParPac.

Digital Rock Generation

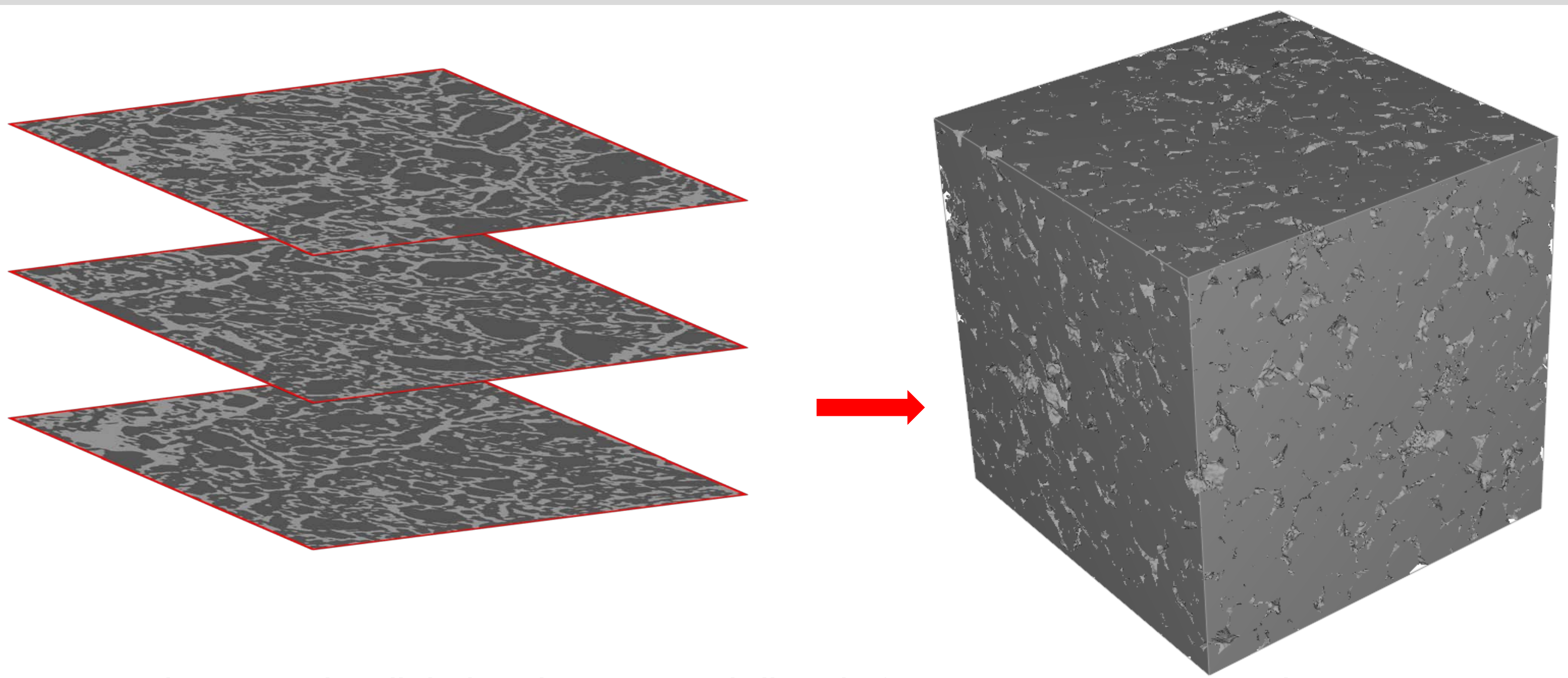

Figure 1: The digital rock generated directly from 3D X-ray tomography.

The lack of detailed knowledge about the rock or soil geometry hinders the understanding of its properties. Computer tomography (CT) can be used to provide detailed spatial information of rock samples.

The Flow Solvers in GeoDict

To predict the permeability of the rock, 3D CFD simulations are performed on a representative segmented CT-image. The flow field is usually obtained by solving the Navier-Stokes equations. In our cases the flows are so slow, that the inertia term in the momentum equations can be neglected. Therefore the Stokes equations are solved. Periodic boundary conditions are applied:

$$\begin{aligned} -\mu\Delta\vec{u} + \nabla p &= 0 \text{ (momentum balance)} \\ \nabla\cdot\vec{u} &= 0 \text{ (mass conservation)} \\ \vec{u} &= 0 \text{ on } \Gamma \text{ (no-slip on fiber surfaces)} \\ P_{in} &= P_{out} + c \text{ (pressure drop is given)} \end{aligned}$$

μ : fluid viscosity,
$\vec{u}$: velocity, periodic,
p : pressure, periodic up to pressure drop in flow direction.

In **GeoDict**, multiple flow solvers are provided.

EJ	**E**xplicit **J**ump immersed interface method. The jump conditions are solved by adding auxiliary forces on obstacles. The jump corrected standard difference formulas are solved with the Fast Fourier Transformation (FFT)[1,2].
SIMPLE	**GeoDict**'s 2012R1 edition **EFV** or **E**xplicit **F**inite **V**olume method. SIMPLE[3] or SIMPLEC[4] algorithm on uniform Cartesian grids.
SIMPLE-FFT	**GeoDict**'s 2012R2 edition **EFV.** FFT- accelerated SIMPLE(C) algorithm. For explicit schemes, the inaccuracy of the pressure correction step is known to require excessively many iterations[5]. An exact implicit solve using the FFT reduces the iteration count at O(n log n) cost.

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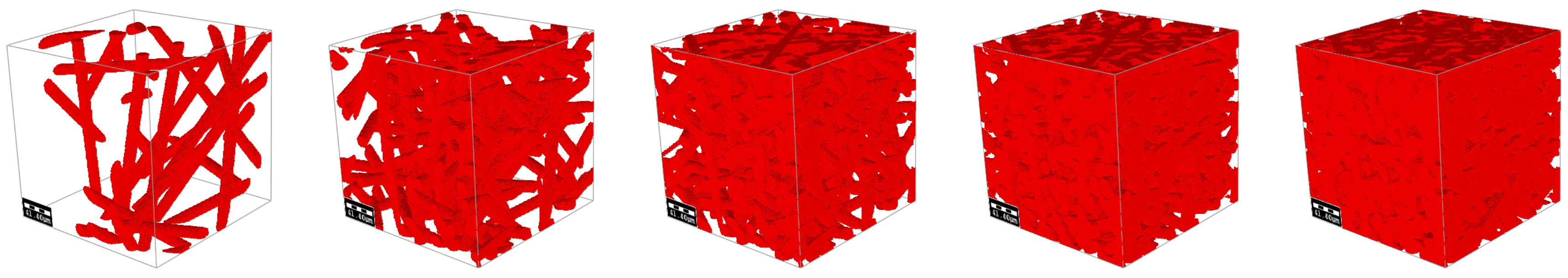
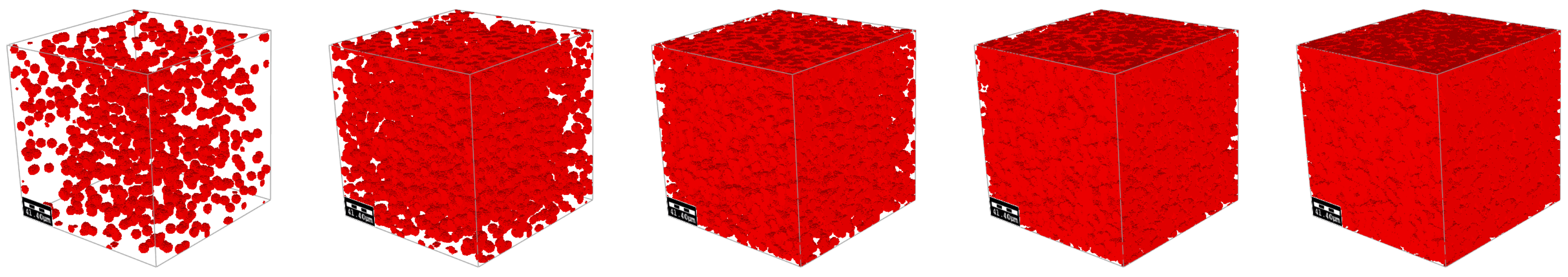
EJ, SIMPLE, and SIMPLE-FFT



9 Fibrous structures sized 200³ with SVF varying from 5% to 75%, 4 realizations per type and porosity



9 Sintered structures sized 200³ with SVF varying from 5% to 75%, 4 realizations per type and porosity

Figure 2: The structures for comparisons of computational performances of EJ, SIMPLE, and SIMPLE-FFT.

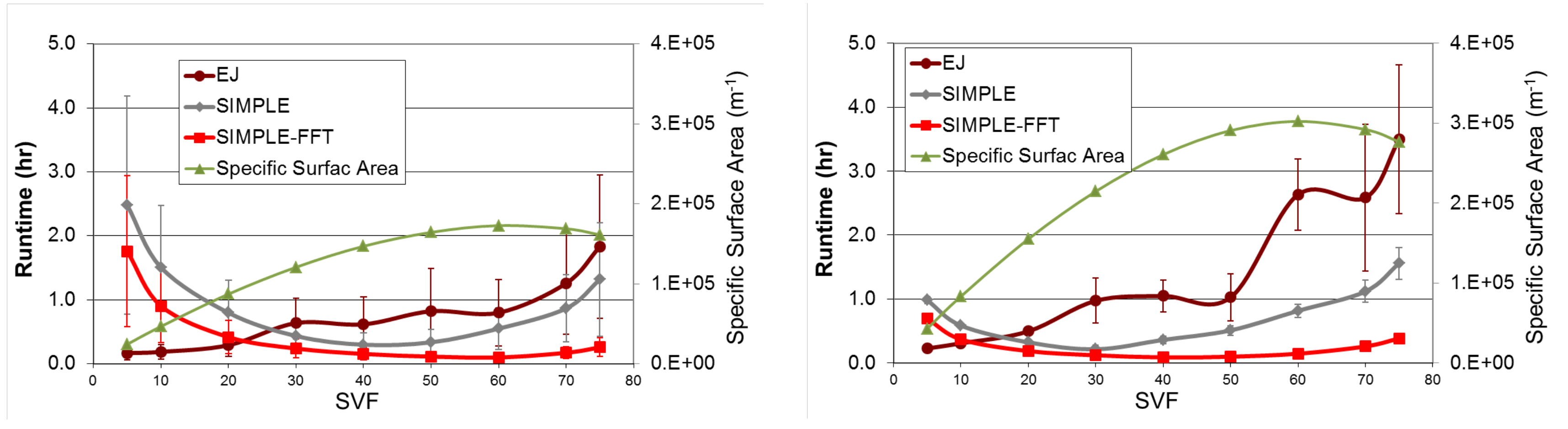


Figure 3: The time costs of EJ, SIMPLE, and SIMPLE-FFT. Computer: Intel(R) Xeon(R) 1.8GHz, 8 core, Memory 64GB, Ubuntu-Linux.

SIMPLE-FFT and ParPac

ParPac is Fraunhofer ITWM's in-house lattice Boltzmann simulation code. It performed better than the 2012R1 edition EFV, SIMPLE, for low porosity materials. The modification to SIMPLE-FFT greatly improved the convergence in the 2012R2 edition, and reduced the runtime significantly, even better than ParPac.

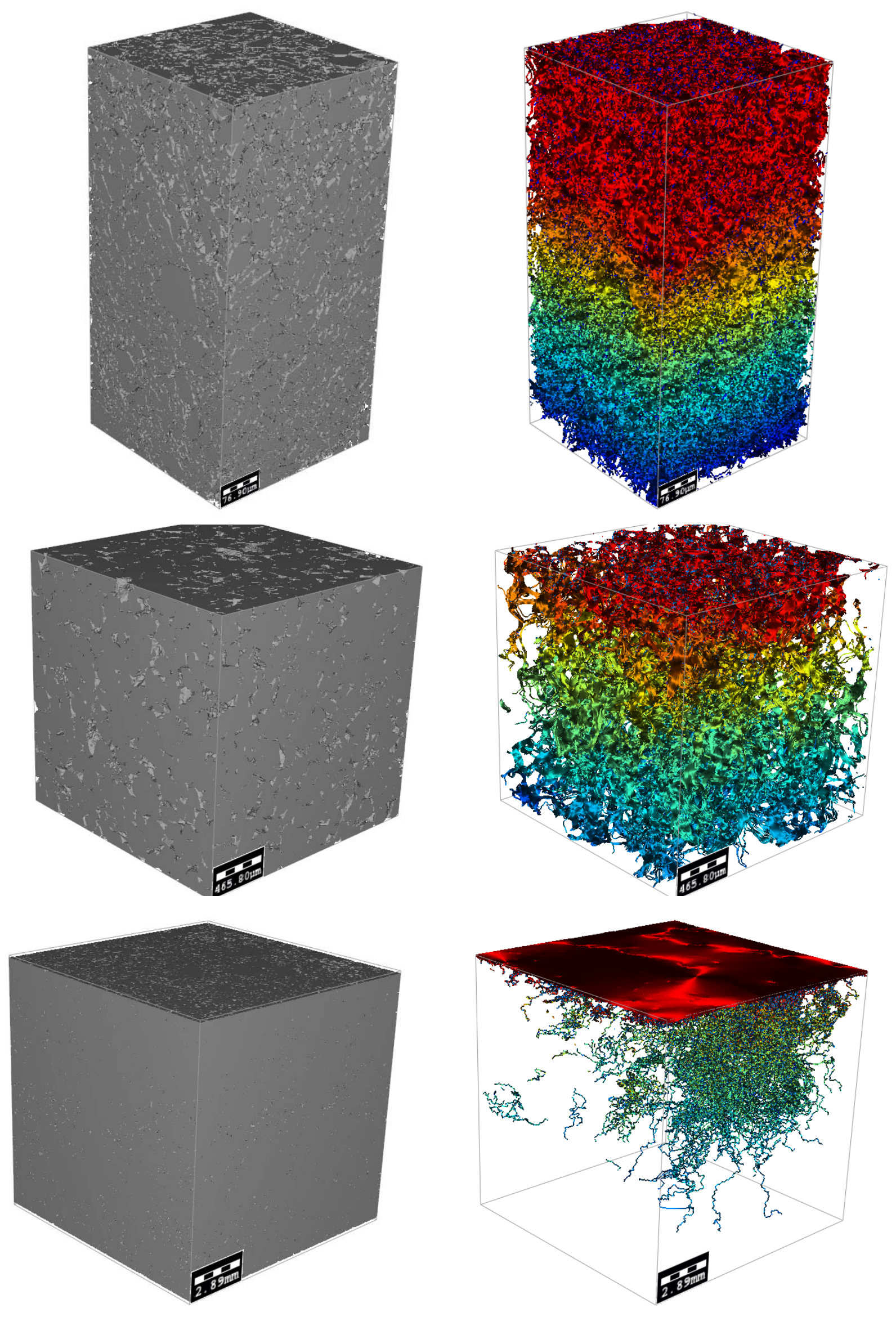


Figure 4: The three rock samples[6] (left) and stream lines (right) with color representing the pressure scale.

Sample 1: Size 500 x 500 x1000; Voxel length 0.74µm; Porosity 33.86%

Sample 1	ParPac				SIMPLE-FFT			
Processes	2	4	8	16	2	4	8	16
PermeabilityZ	1.230E-13				1.145E-13			
Runtime (hr)	20	14	4.4	2.5	3.5	2.5	1.1	0.6
Memory (GB)	88	92	104	123	20	21	22	23

Sample 2: Size 750 x 750 x 750; Voxel length 2.99µm; Porosity 17.72%

Sample 2	ParPac				SIMPLE-FFT			
Processes	2	4	8	16	2	4	8	16
PermeabilityZ	8.013E-13				7.665E-13			
Runtime (hr)	26	15	4.5	6.5	9.5	4.7	3.5	2
Memory (GB)	133	140	150	168	34	35	36	37

Sample 3: Size 512 x 512 x 512; Voxel length 27.1µm; Porosity 16.72%

Sample 3	ParPac 8 procs	ParPac 16 procs	SIMPLE-FFT 8 procs	SIMPLE-FFT 16 procs
PermeabilityZ	diverge	diverge	2.509E-13	2.509E-13
Runtime (hr)	inf	inf	48	40
Memory (GB)	51	60	11	15

Table 1, 2, 3: Comparisons of ParPac and SIMPLE-FFT with respect to results, runtime and memory cost. AMD Opteron 1.4GHz, 64 core, Memory 512GB, Scientific Linux

Conclusions

- SIMPLE-FFT exhibits greatly improved convergence. Especially for low porosity structures, the speedup is up to 10 times faster compared to the code 2012R1 code used e.g. in [7].
- EJ performs best when the structure has low solidity and low specific surface area, less than 20% solidity for fibrous structures and less than 10% solidity for sintered structures.
- SIMPLE-FFT runs faster and stabler than ParPac. By adding more processors from 8 to 16 may not help to speed up the computations of ParPac (see sample 2), but does for EFV.

References

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