Parallelising the Monte Carlo simulation of THz conductivity

<u>Nikolay N. Reutskii</u>[1], Egor A. Nikulchin[2],Vladislava V. Bulgakova[2], Pavel A. Chizhov[2], Alexander A. Ushakov[2], Roman Y. Pishchalnikov[2]

[1]Lomonosov Moscow State University, Faculty of Physics, Moscow

[2]Prokhorov General Physics Institute
of the Russian Academy of Sciences, Moscow

Outline

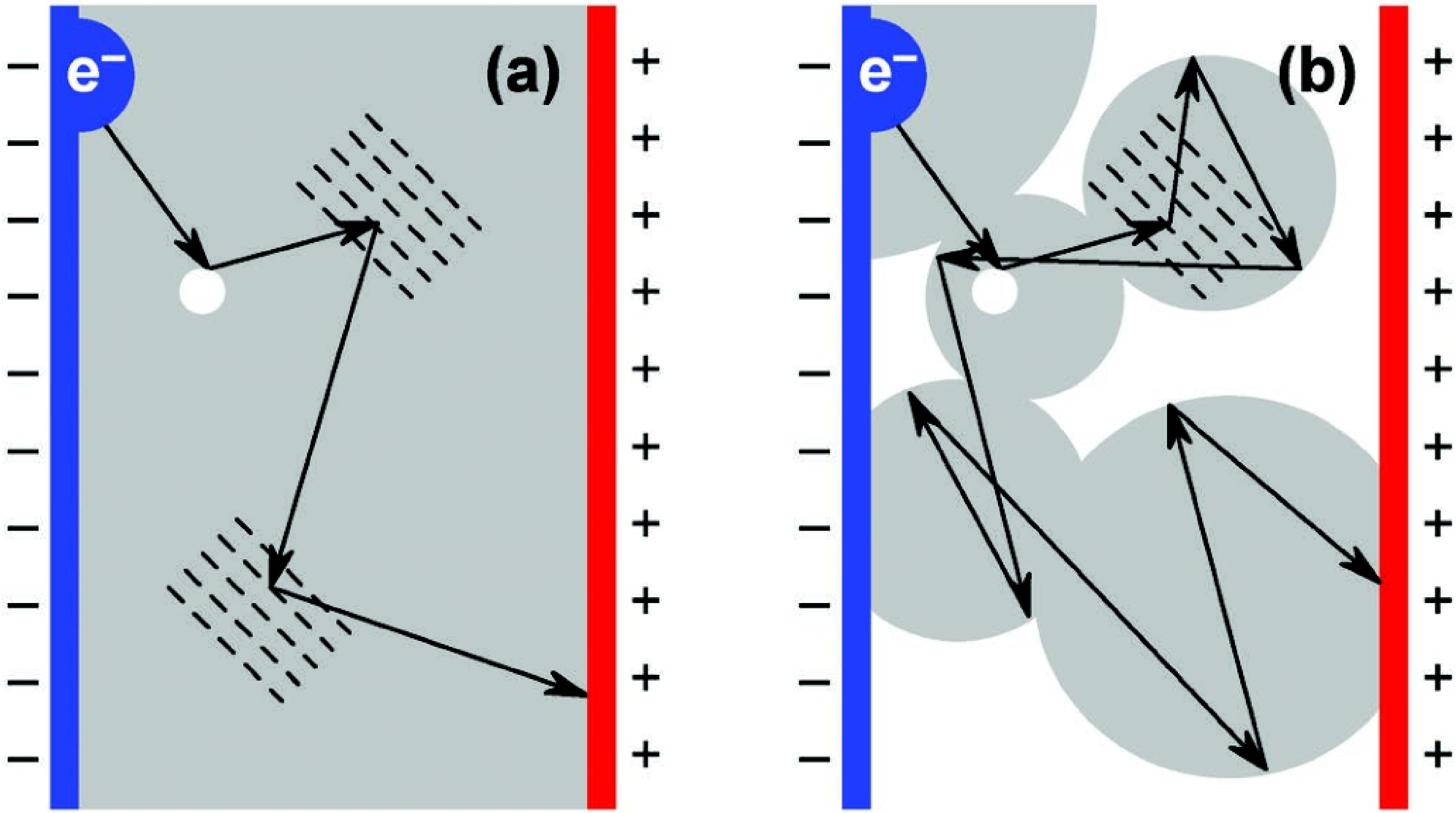
1. ***THz conductivity in nanomaterials***
2. ***Parallelization of the algorithm***
   - ***Integration algorithms***
   - ***Spatial / Temporal parallelisation***
3. ***Achieved results***
4. ***Summary and areas to improve***

THz conductivity

Wide range of applications:

- ***Transparent electrodes in displays and solar cells***
- ***Quantum Dots***
- ***Nanocomposites***
- ***Spectroscopy***
- ***… the list goes on***

Simulation algorithm



Simulation algorithm

$$\sigma(\omega) = \sigma_1(\omega) + \sigma_2(\omega) = \frac{\sum_{k=\overline{1,M}} \langle v_y(0), v_y(t_k)\rangle e^{i\omega t_k}}{\sum_{l=\overline{1,M}} \cos \omega t_l e^{i\omega t_l}}$$

Integration methods

1. *Forward Euler and Backward Euler*
2. *Runge–Kutta 4*
3. *Velocity Verlet*
4. *Leapfrog*

Naïve spatial parallelisation — OpenMP

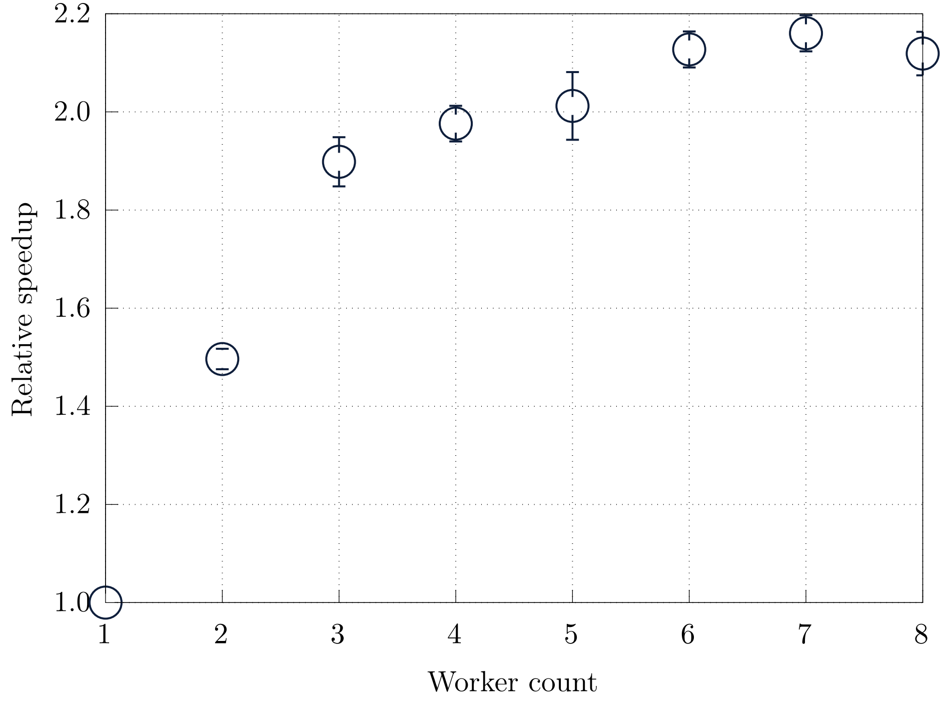
Pros:

- ***Ease of transition from serial to parallel***
- ***Wide compiler support for*** `omp #pragma`***s***

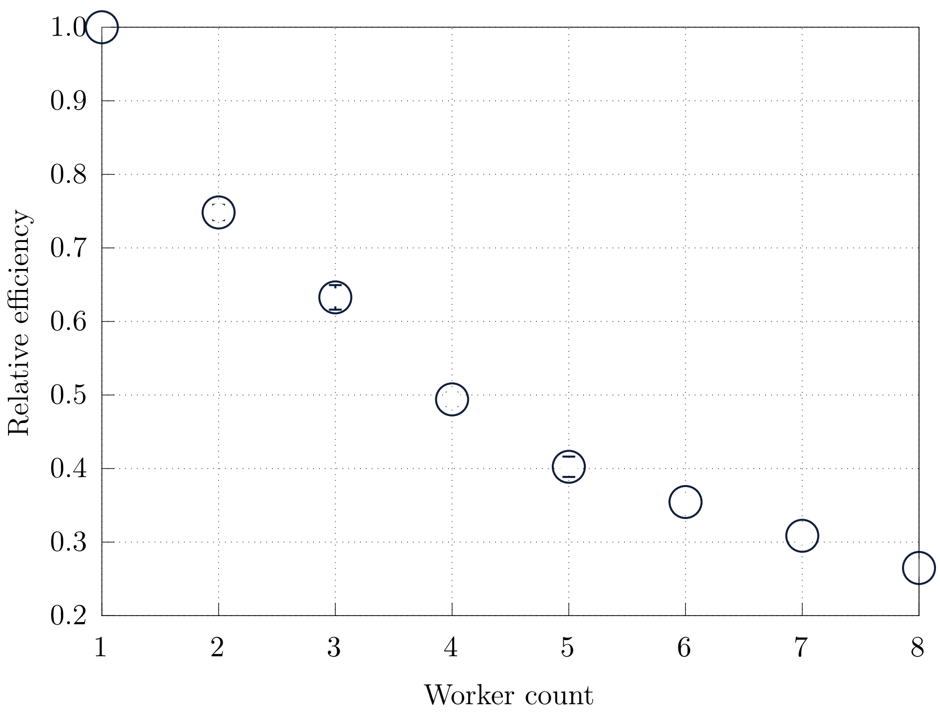
Cons:

- ***Codegen causes difficult debugging***
- ***Less robust than solutions like MPI***

Results



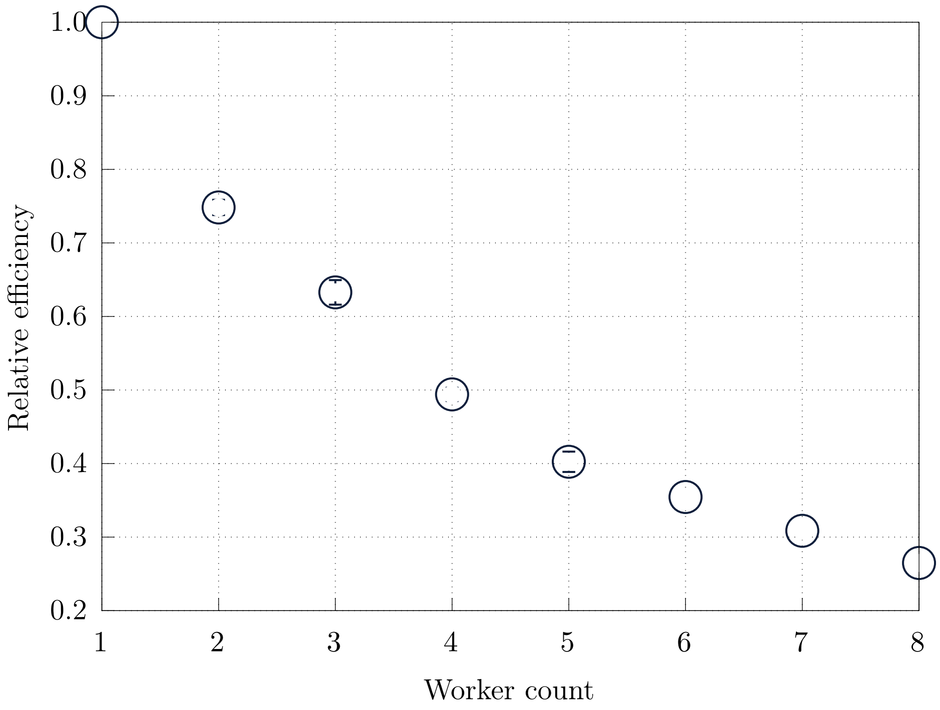
Relative speedup
2.2
2.0
1.8
1.6
1.4
1.2
1.0
1
2
3
4
5
6
7
8
Worker count



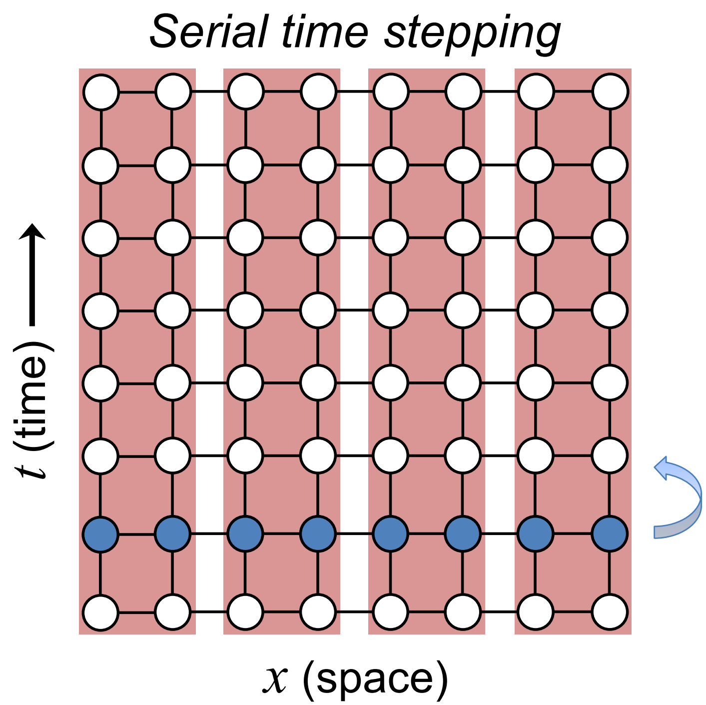
Relative efficiency
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
1
2
3
4
5
6
7
8
Worker count

Results

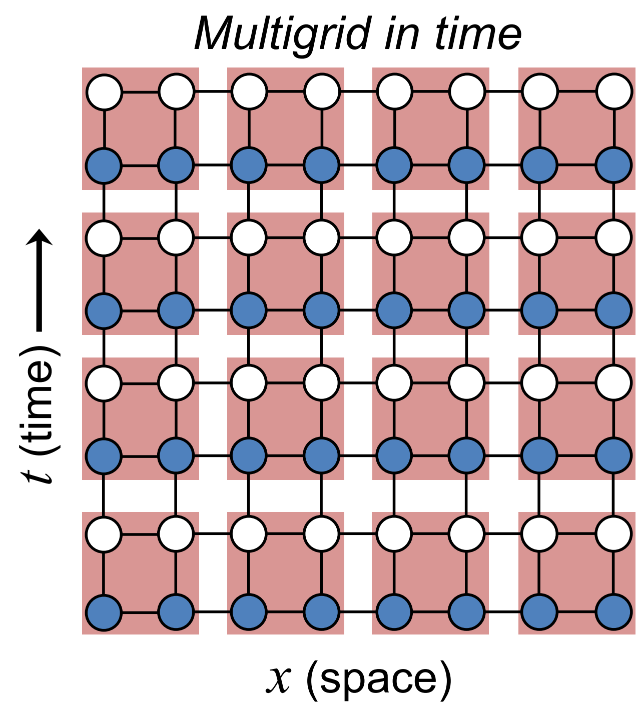
Time integration becomes the bottleneck



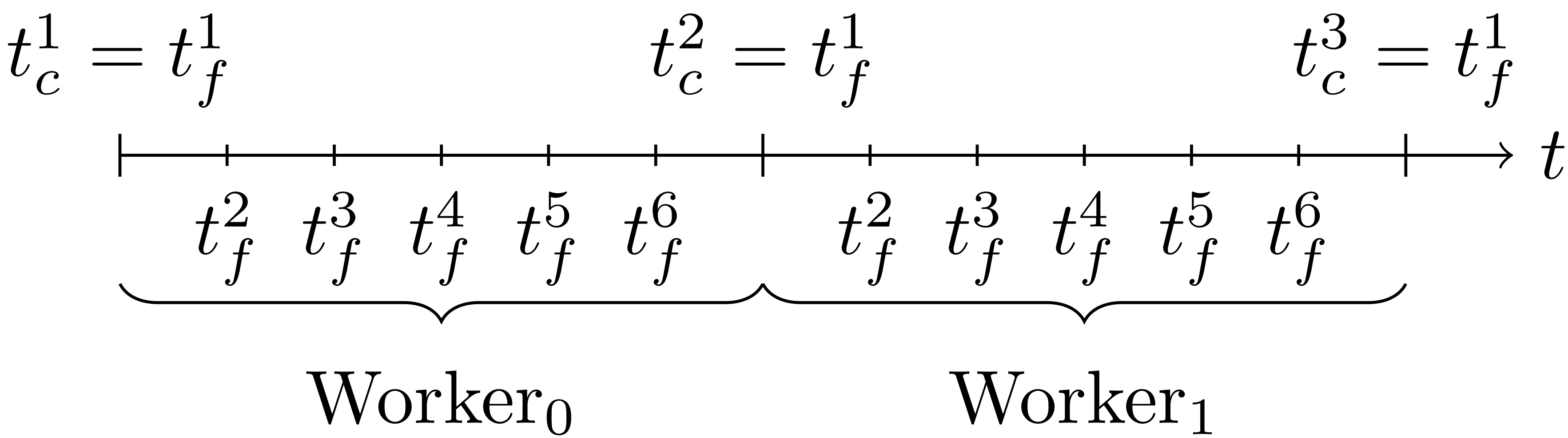
Eliminating the bottleneck — MGRIT



C



Temporal parallelisation — MGRIT



Temporal parallelisation — MGRIT

- ***Xbraid***
- ***C/C++***
- ***«Black box» API***

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of Prokhorov General Physics Institute
of the Russian Academy of Sciences, Moscow

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