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Data compression and parallelization in simulations of transient regimes

Jeremija Kovačević

Scientific Computing Laboratory Center for the Study of Complex Systems Institute of Physics Belgrade Belgrade, Serbia

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Motivation

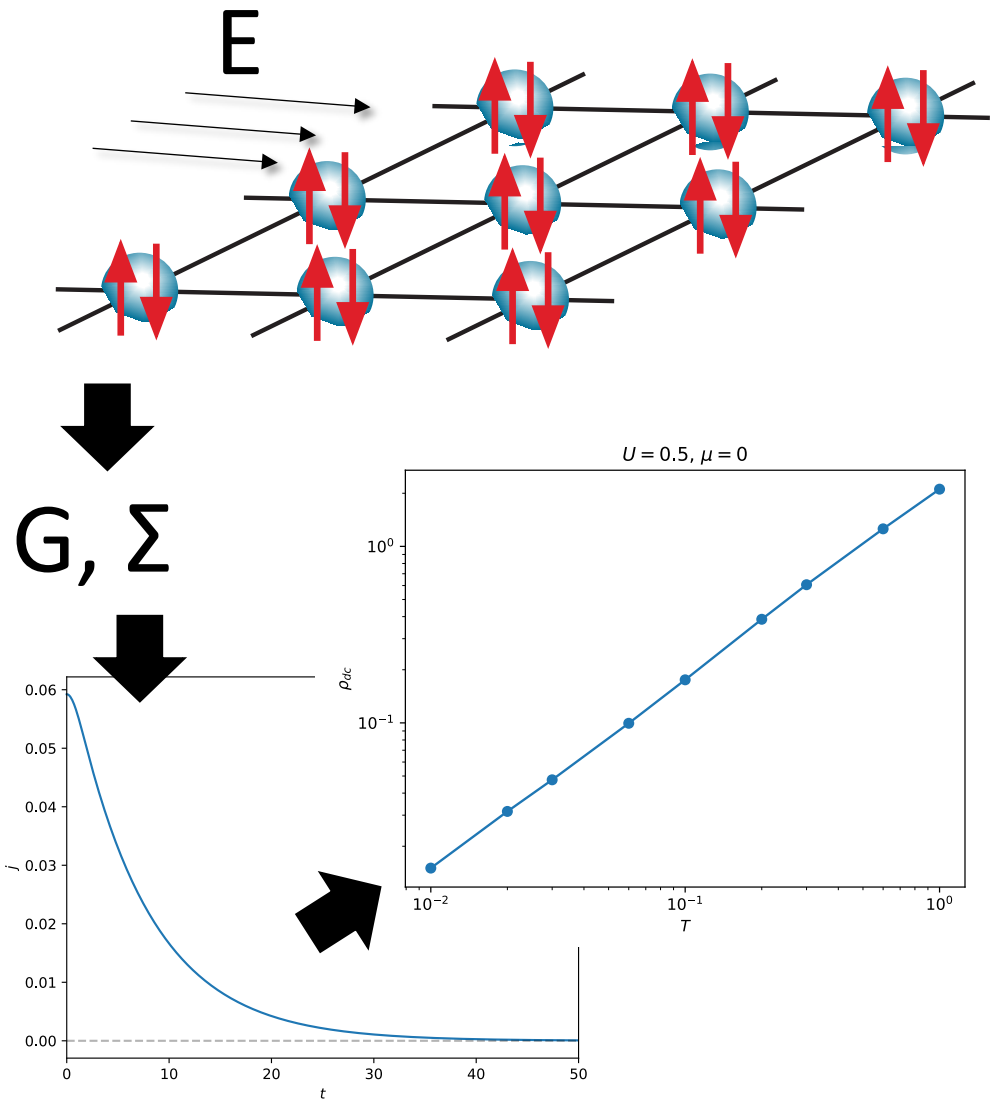
- Our goal is to understand and predict the physical and electronic properties of materials
- Central quantities of interest are the dynamical response functions, particularly electrical conductivity

$$X_i(\mathbf{r},t) = \int d^d r' \int dt'\, \chi_{ij}(\mathbf{r},t;\mathbf{r}',t') F'_j(\mathbf{r}',t')$$

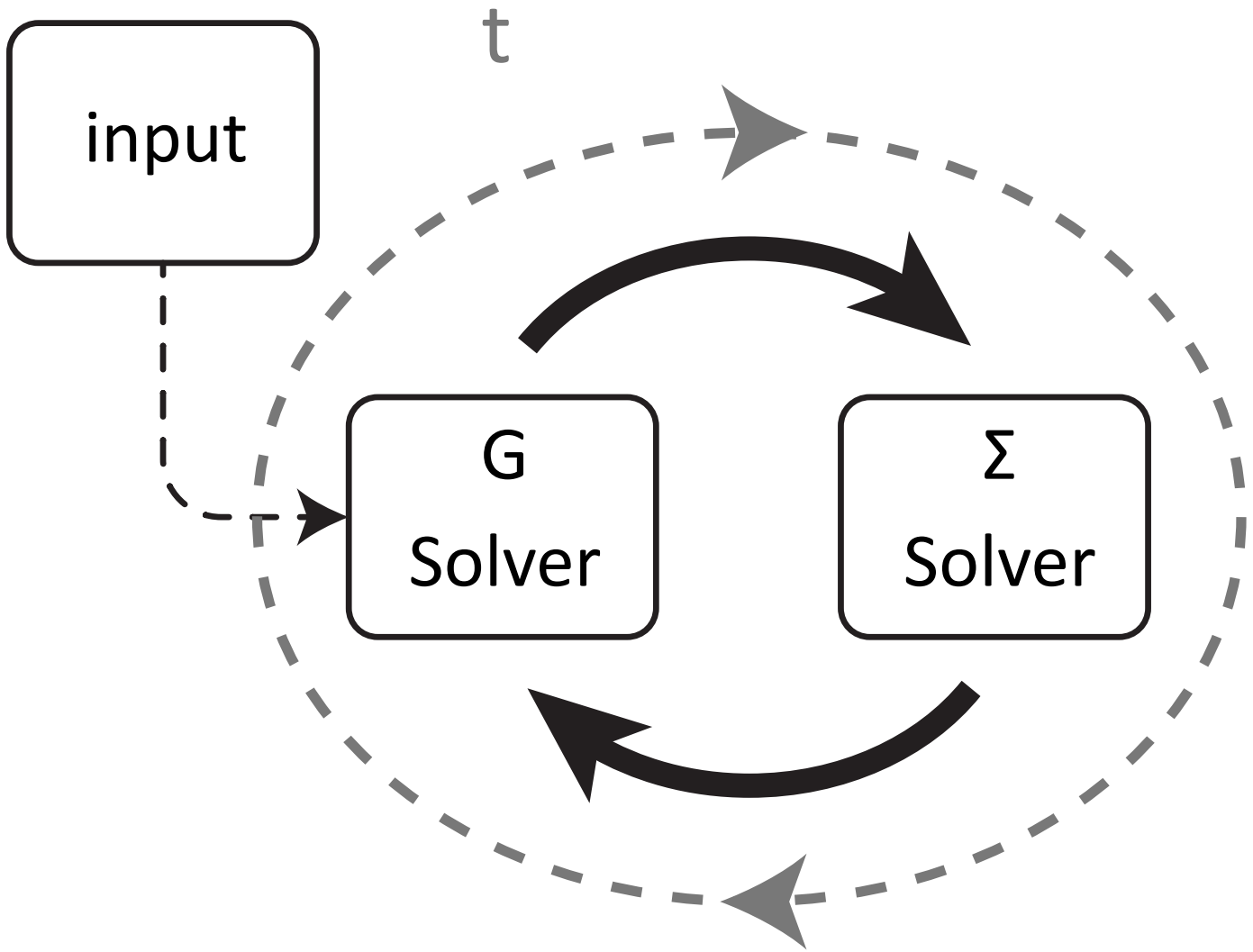
- Dynamical response functions encode the intrinsic properties of the system
- In equilibrium, calculate dynamical response function directly (no transient regimes)
- In Non-equilibrium, Probing the models with external fields and calculating the response

What we do

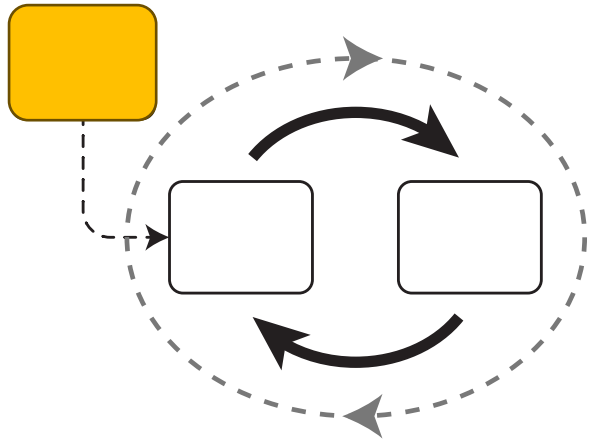
- Simulate an electron system on a lattice under a short electric pulse E
- Compute the Green's function $G_r(t,t')$: how electrons propagate over time
- Compute the self-energy $\Sigma_r(t,t')$: how interactions modify propagation
- Calculate current j from G
- Extract conductivity form the current
- Vary physical parameters (T, U, μ)
- Two natural domains: site space and k-space



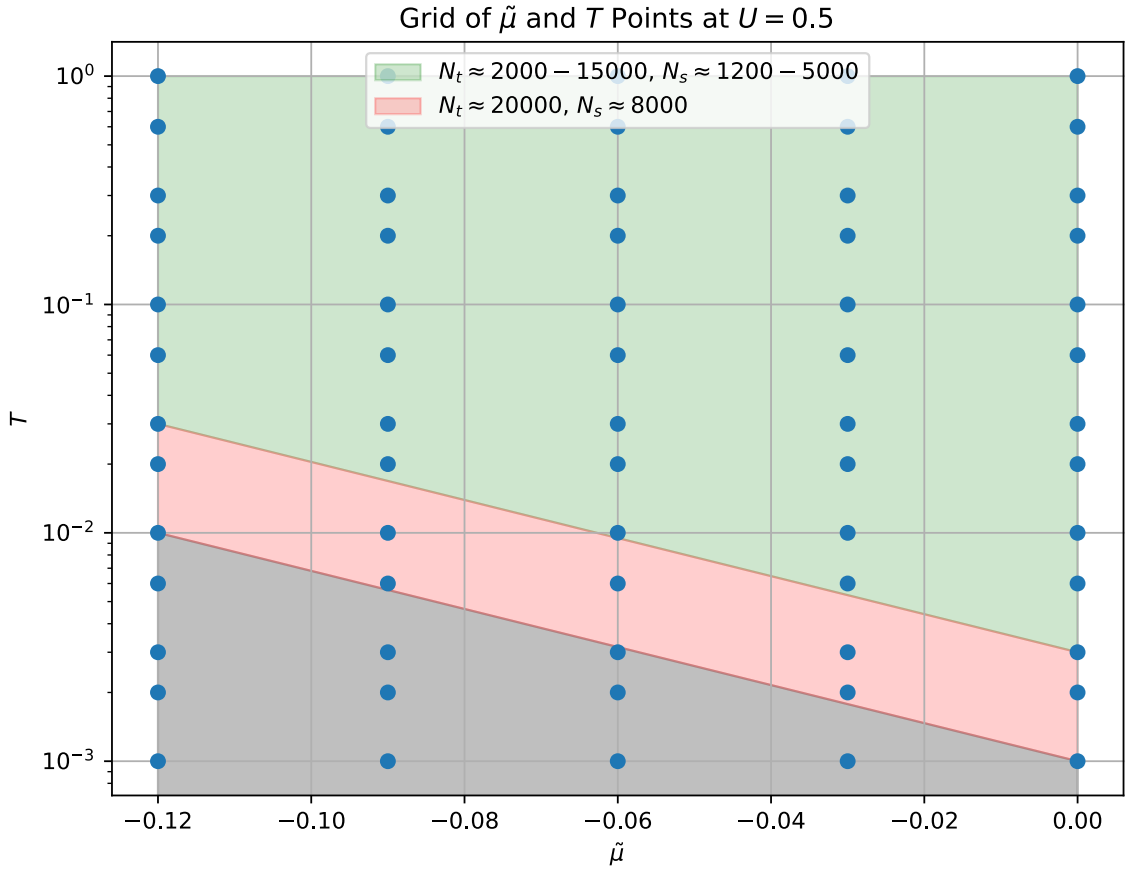
Algorithm



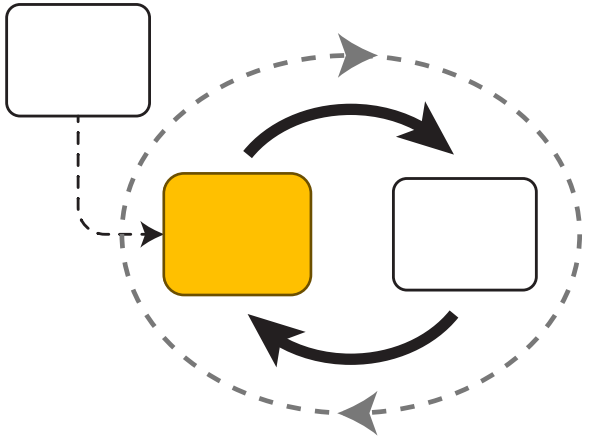
Input



- Temperature T
- Interaction strength U
- Doping level μ
- Lattice type
- Number of lattice sites N_s
- Number of time points N_t
- Time step discretization Δt
- Profile of the electric field pulse



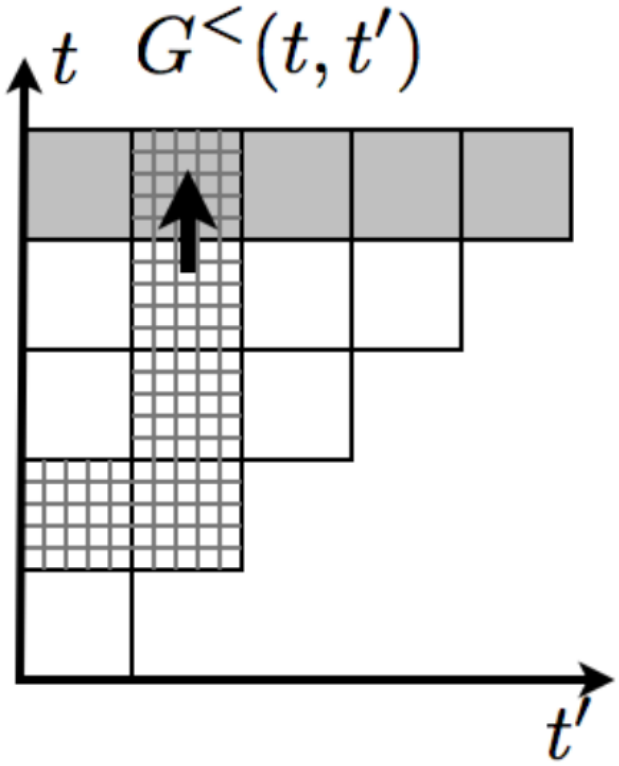
Calculating G



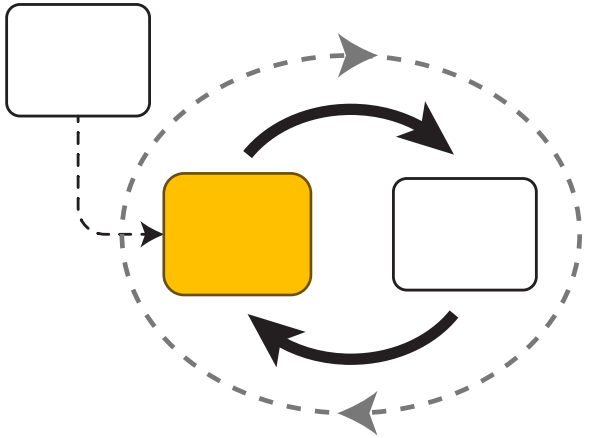
- Kadanoff-Baym equations (KBE)

$$i\partial_t G_{\mathbf{k}}(t,t') = \varepsilon_{\mathbf{k}}(t) G_{\mathbf{k}}(t,t') + \int_0^t \mathrm{d}\bar{t}\, \Sigma_{\mathbf{k}}(t,\bar{t}) G_{\mathbf{k}}(\bar{t},t')$$

- Self-consistent equations
- Time-stepping algorithm
- History integrals require knowledge of G and Σ for all times
- Embarrassingly parallel over k points
- NESSi (Computer Physics Communications 257, 107484 (2020))



Scaling of the KBE Solver

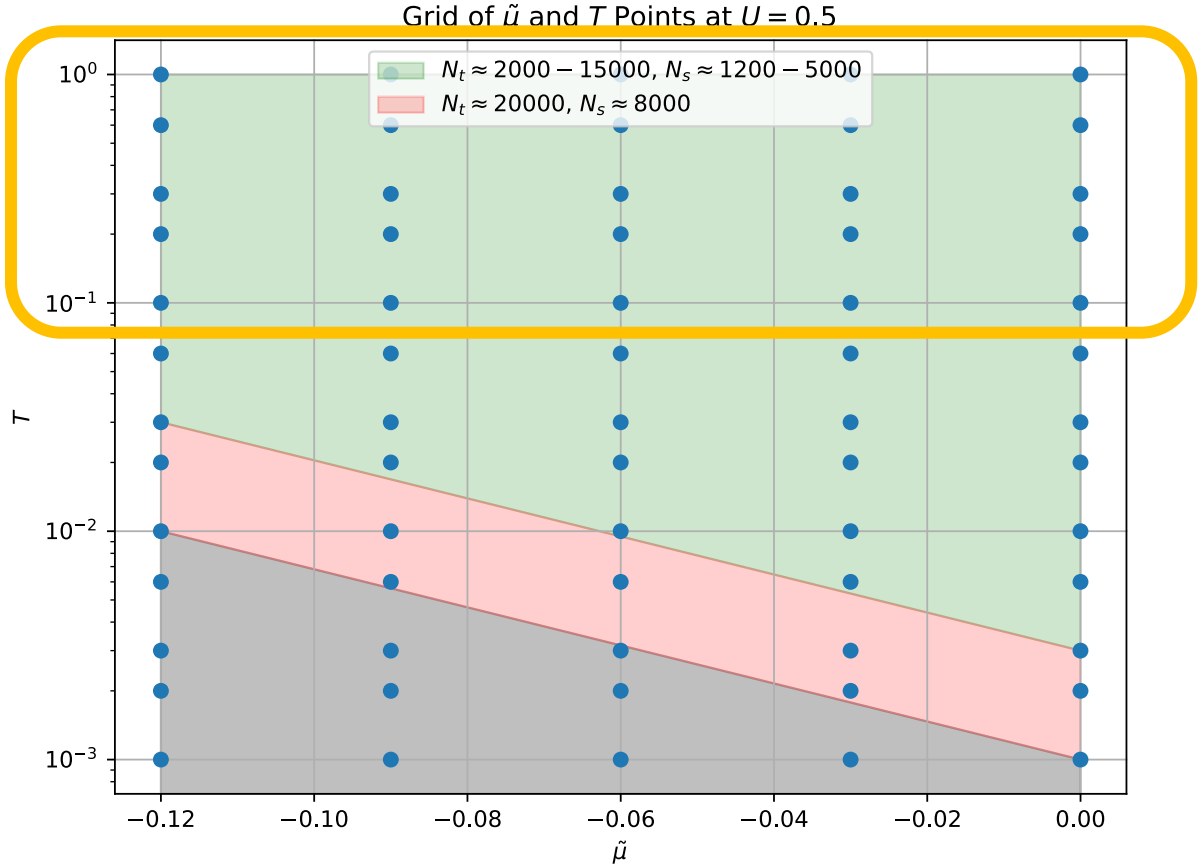


$$i\partial_t G_{\mathbf{k}}(t,t') = \varepsilon_{\mathbf{k}}(t) G_{\mathbf{k}}(t,t') + \int_0^t \mathrm{d}\bar{t}\, \Sigma_{\mathbf{k}}(t,\bar{t}) G_{\mathbf{k}}(\bar{t},t')$$

- Memory cost of G and Σ

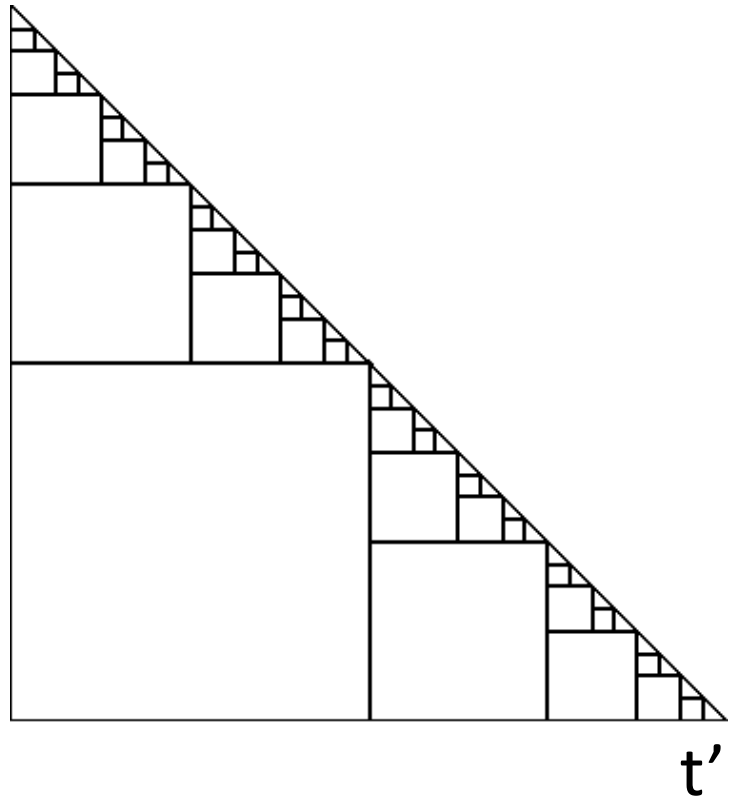
  $N_t = 10000$, $N_s = 5000$

  $2 \times N_t^2 \times N_s \times 16\mathrm{B} \approx 15\ \mathrm{TB}$
- Computational cost scales as N_t^3
- Large part of the parameter space is unavailable



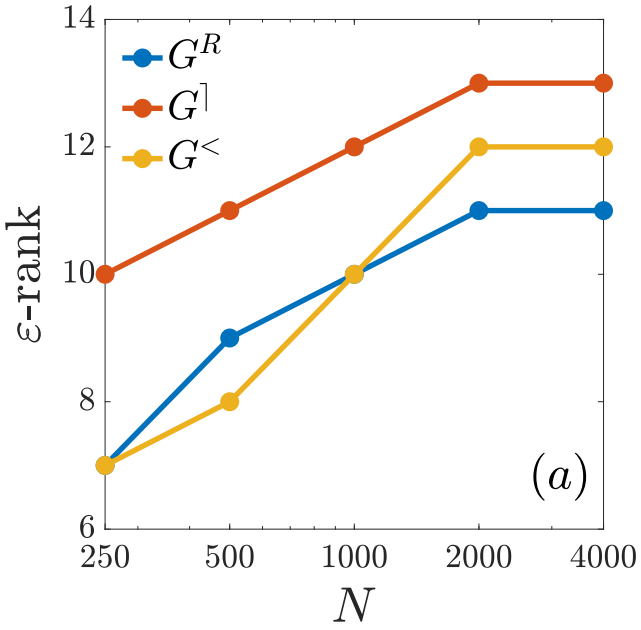
Data compression with SVD

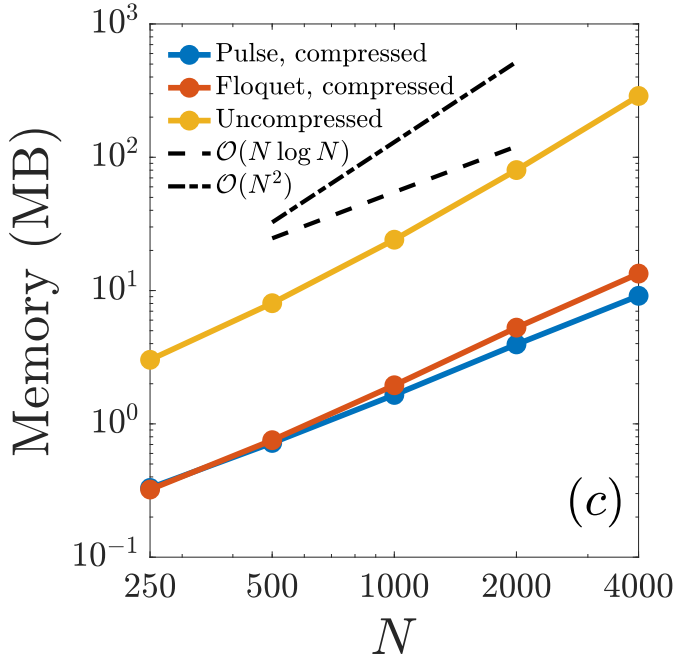
- Key Idea: Far from the diagonal there is less and less information
- In that region there should be a low-rank representation
- Hierarchically off-diagonal low-rank (hodlr)
- Small control parameter to control the scaling
- Matrix partition and perform SVD on each block
- We never save all the blocks, just their SVD representation



Data compression with SVD

- Ranks of blocks are much smaller than N and grow weakly with N
- Memory usage grows logarithmically
- History integrals are evaluated with SVDs which reduces costs
- Reduction of computational cost $N^3 \rightarrow N^2 \log(N)$
- Memory requirements $N^2 \rightarrow N \log(N)$
- Example: 5 months, 2.2TB → 26.5h, 3.8GB
- Lossy compression
- We don't know RAM usage ahead of time
- hodlr (SciPost Phys. 10, 091 (2021))





Self-Energy calculation

- KB solver operates naturally in k-space
- Cost of Σ calculation:

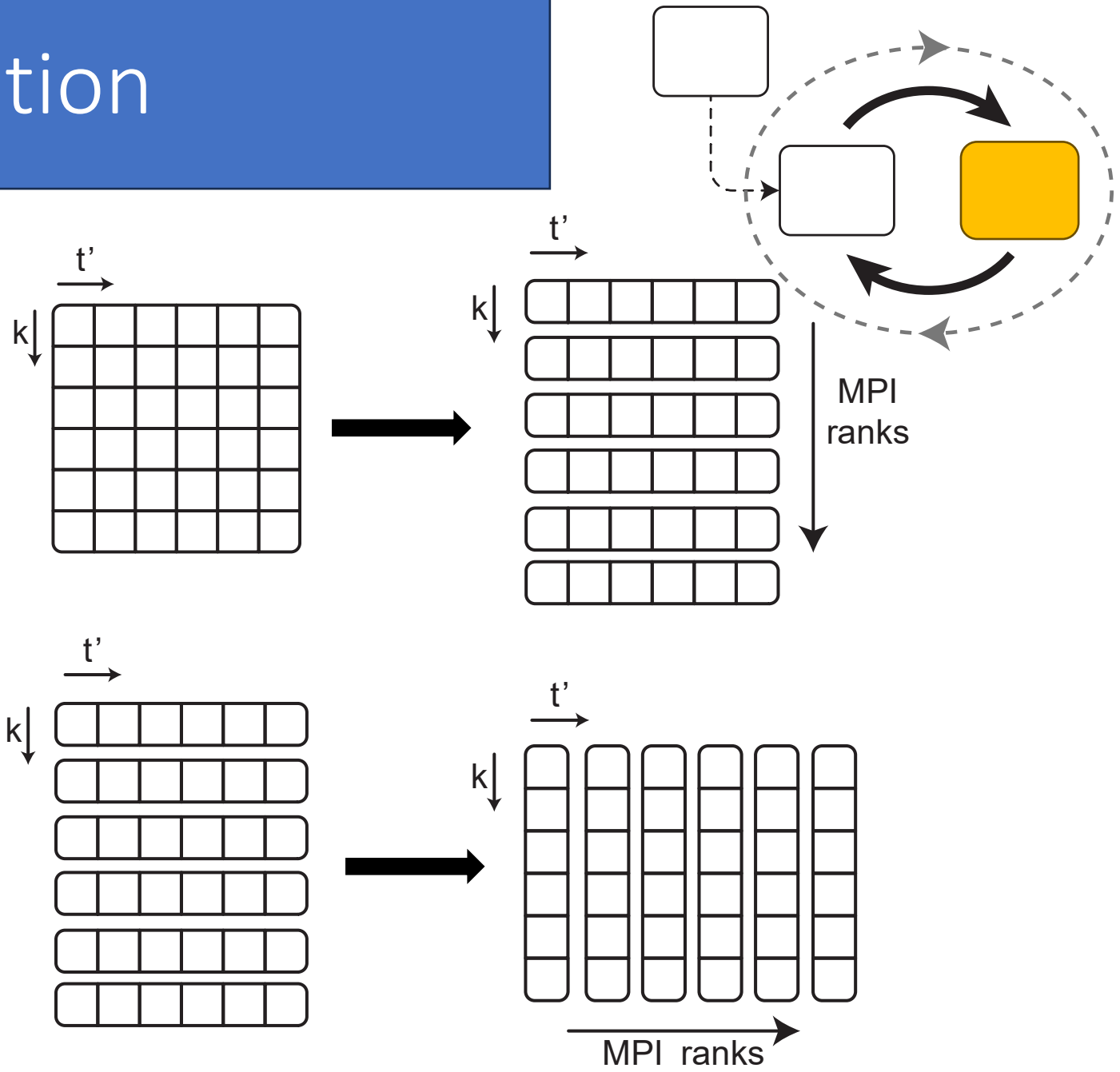
  $O(N_s^3)$ in k-space

  $O(N_s)$ in site space
- Cost of a Fourier transform:

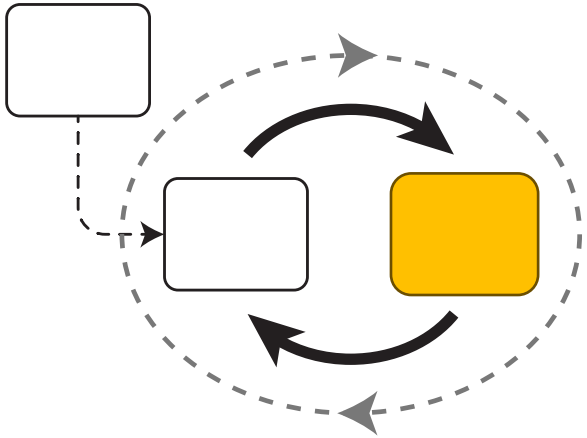
  $O(N_s \log(N_s))$
- A way to go:

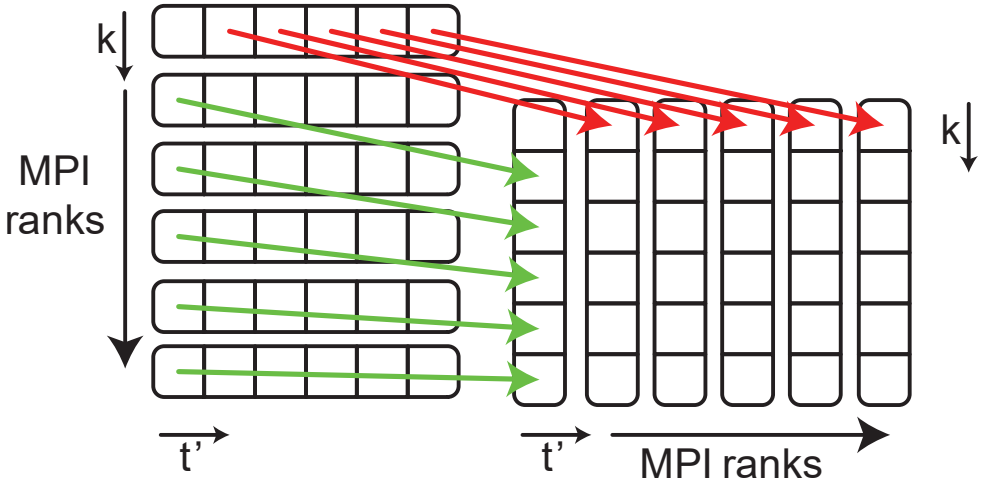
  $G_k \rightarrow G_r \rightarrow \Sigma_r \rightarrow \Sigma_k$

  $O(N_s \log(N_s))$



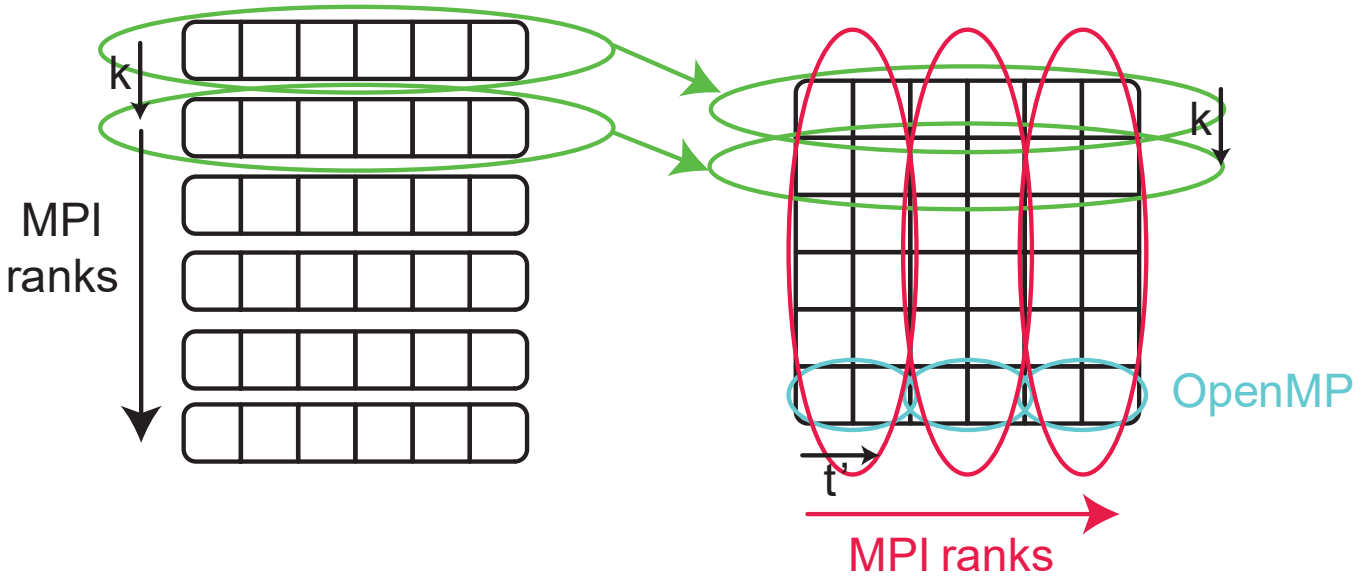
Parallelization strategies





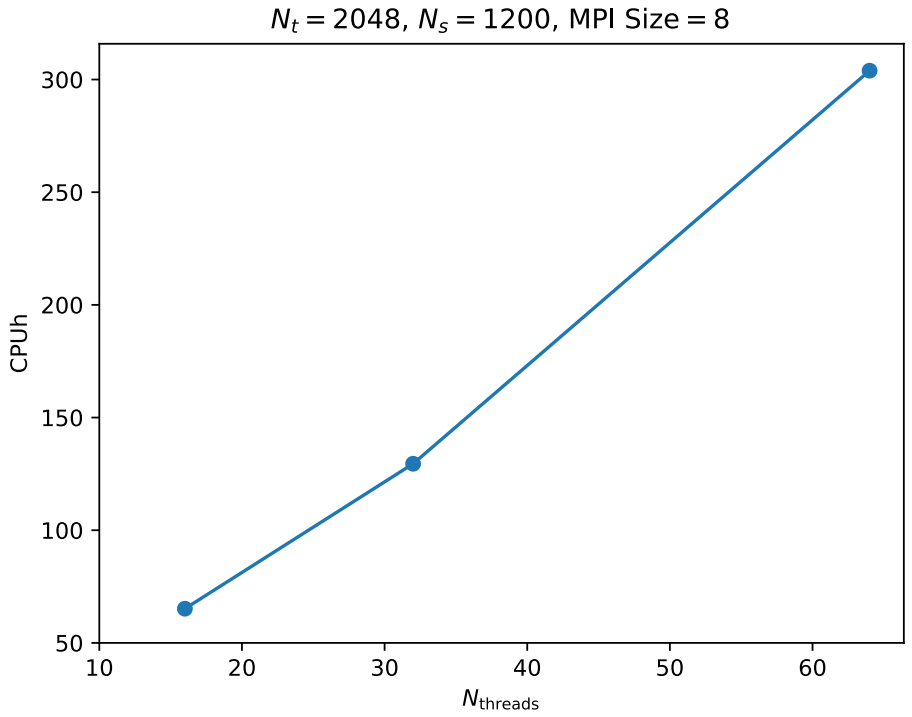
- MPI Send and Receive
- Simple to implement
- Too many communications

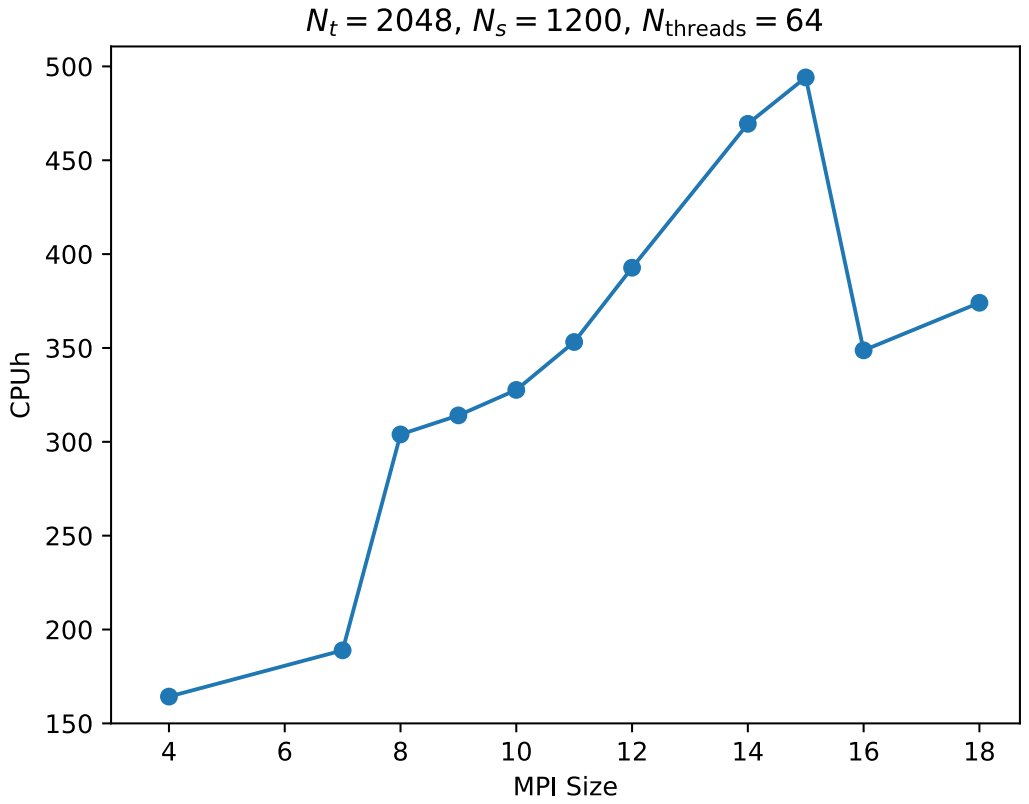
- MPI gather + OpenMP
- Harder to implement
- Less communications
- Better scaling



Scaling with MPI size and thread count

- Complicated scaling
- MPI communications become a bottleneck
- Threads are wasted





- Spawning threads can be costly

Summary and Conclusions

- We computed G and Sigma in the Kadanoff-Baym formalism to extract conductivity in the interacting electron system.
- Two-time nature of the problem leads to huge memory and computational costs.
- Our block-wise SVD compression reduces memory and computational complexity dramatically.
- Using FFT we switch between site and momentum space optimizing different parts of the calculation.
- Hybrid MPI+OpenMP offers complicated but better scaling options.