ICTP Advanced School on Scientific Software Development Project:

Parallel Implementation of Typical Medium Theory

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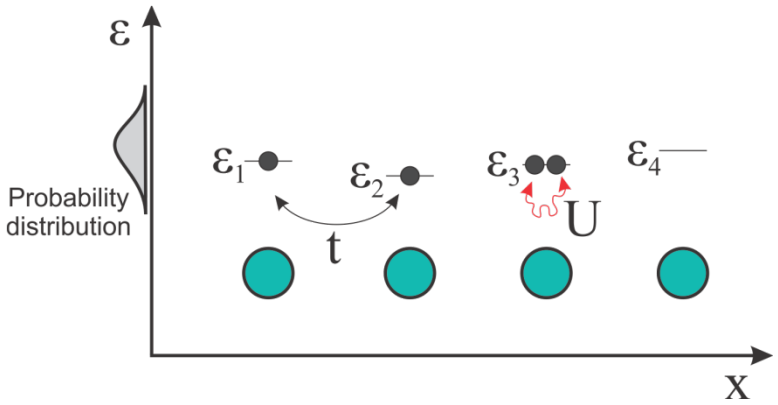
Fields of interest: condensed matter theory, strongly correlated electronic systems

Main research topic: dynamical mean field theory

- Typical medium theory (TMT)
  - A method of solving the infinitely-dimensional disordered Hubbard model



  - First proposed bv V. Dobrosavlievic in 2003

Typical medium theory of Anderson localization: A local order parameter approach to strong disorder effects

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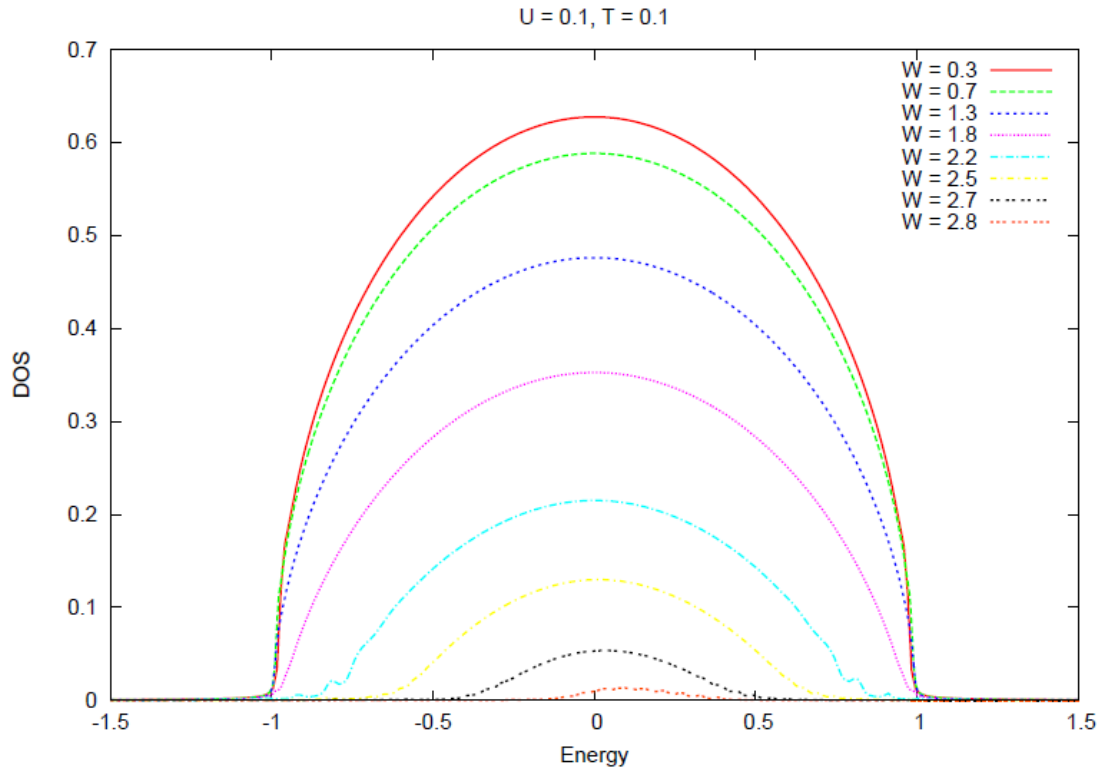
PACS. 72.15.Rn – Localization effects (Anderson or weak localization).
PACS. 71.27.+a – Strongly correlated electron systems; heavy fermions.
PACS. 71.30.+h – Metal-insulator transitions and other electronic transitions.

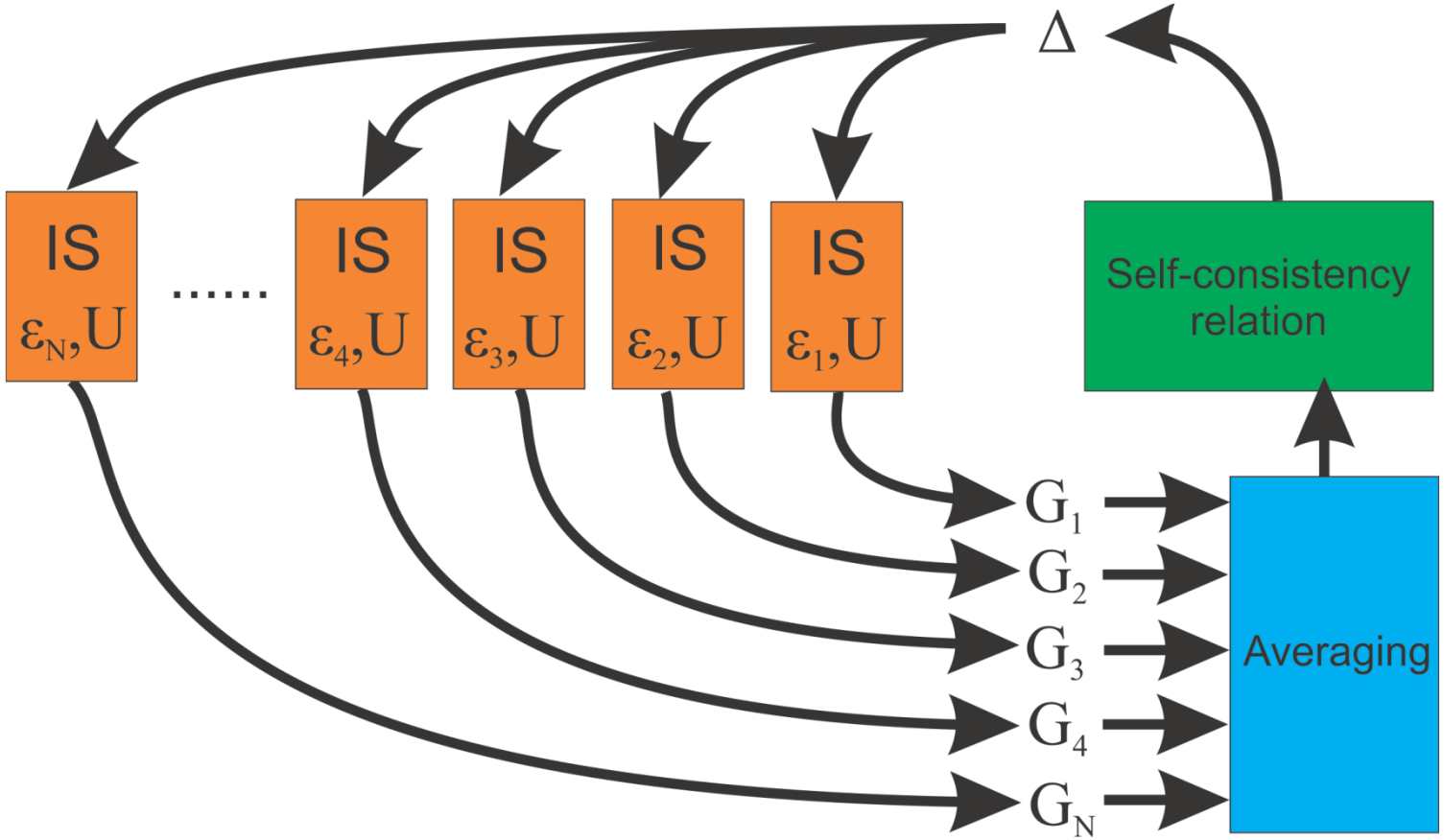
Abstract. – We present a self-consistent theory of Anderson localization that yields a simple algorithm to obtain *typical local density of states* as an order parameter, thereby reproducing the essential features of a phase-diagram of localization-delocalization quantum phase transition in the standard lattice models of disordered electron problem. Due to the local character of our theory, it can easily be combined with dynamical mean-field approaches to strongly correlated electrons, thus opening an attractive avenue for a genuine *non-perturbative* treatment of the interplay of strong interactions and strong disorder.



- Previous results – only for the non-interacting case
  - Strong disorder drives the system into an insulating state by reducing the density of states available to electrons at the Fermi level (Anderson localization)
- We intend to use U>0 and obtain conductivity as a funtion of disorder, interaction strength and temperature

$$\sigma(W,U,T)$$

- Many impurities with randomized orbital energies are considered
- Iterative procedure is repeated until geometrically averaged (typical) impurity Green's function G is consistent with the hybridization function Δ
- My task was to write and parallelize this code so that it can be run in a reasonable time frame



- C++ (around 3000 lines incl. .h files)
- 2 computational nodes of 8 cores (Intel Xeon E5405 @ 2.00GHz) interconnected by Infiniband
- Intel compiler (icpc)
- Hybrid implementation
  (OpenMPI + Intel OpenMP)

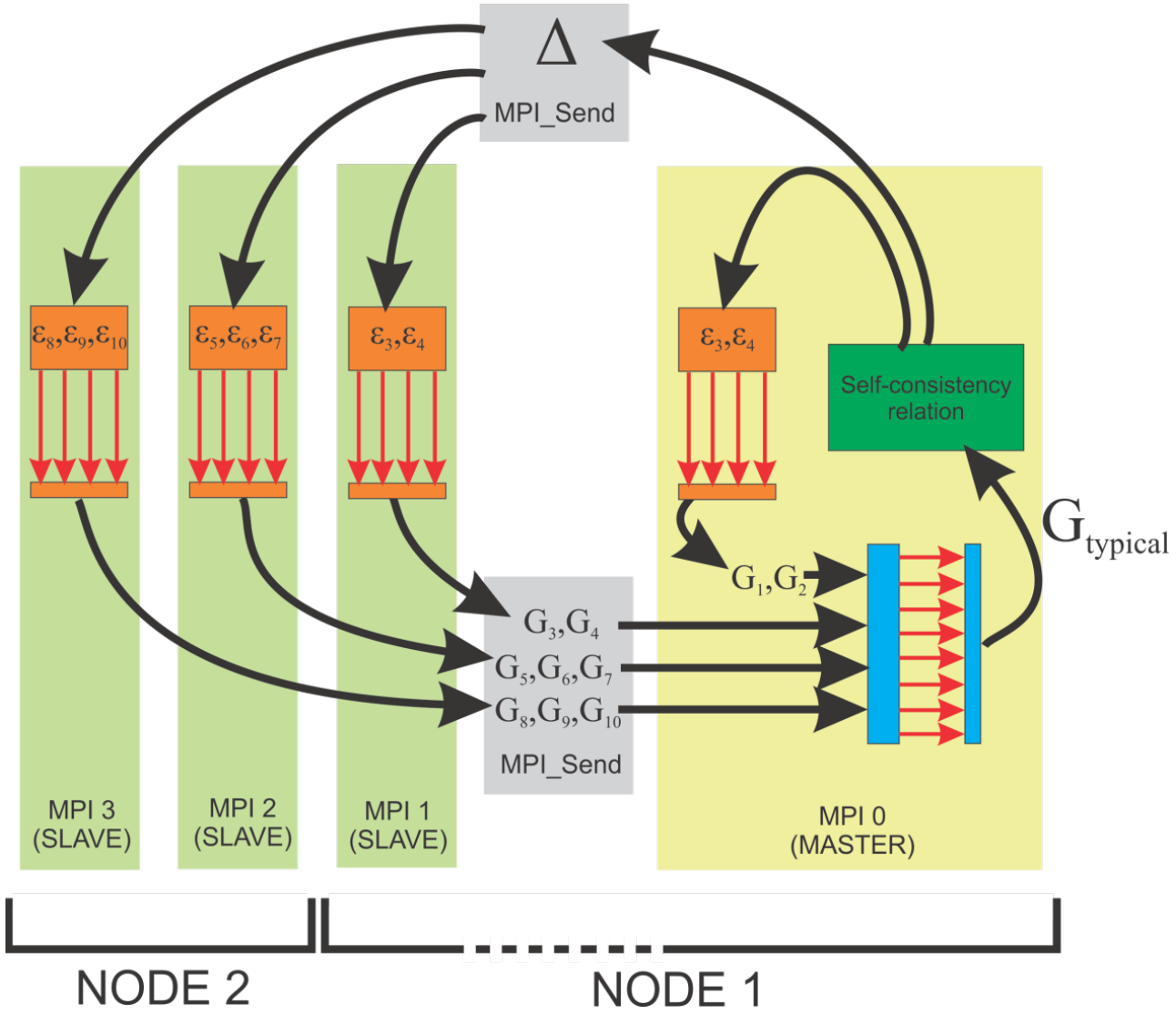
- Example:
  - 4 MPI processes
  - 4 OpenMP threads per MPI process
  - solving 10 impurities

-Impurities distributed equally among MPI processes

-Impurity Solvers parallelized using OpenMP threads solve one impurity at a time

-Averaging performed with 8 threads by master process

-MPI_Send and MPI_Recv used for communication



- Performance test
- Example
  - 32 impurities, U=0.1, T=0.1, W=0.3
  - Functions discretized on a grid of 2000 points
  - 41 iterations needed for reaching convergence

Number of MPI processes	Number of OpenMP threads per MPI process	Execution time [min:sec]
1	1	31:01
1	2	15:46
1	4	07:58
1	8	04:06
16	1	02:20
8	2	02:10
4	4	02:08
2	8	02:07