Next Generation Multi-Scale Quantum Many-Body Simulation Software

Cengiz Sen
University of Cincinnati, effective August 2007

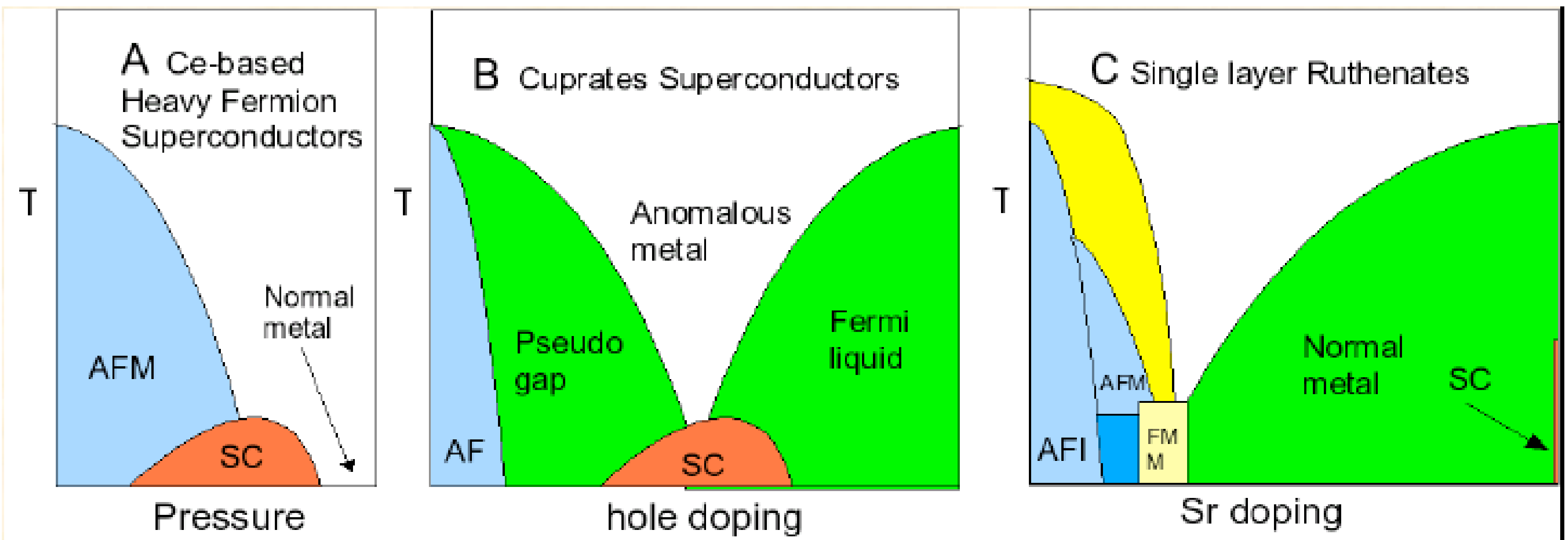
Collaborators:
M. Jarrell, K. Tomko, Th. Maier, E. D'Azavedo, R. Scalettar, Z. Bai, S. Savrasov

OUTLINE

- Complexity at the nanoscale
- Present Approach
  - Improved cluster solvers at short-length scales
- Multi-Scale Many-Body Approach
  - Separation of length scales
  - Diagrammatic methods at intermediate-length scales
- Summary

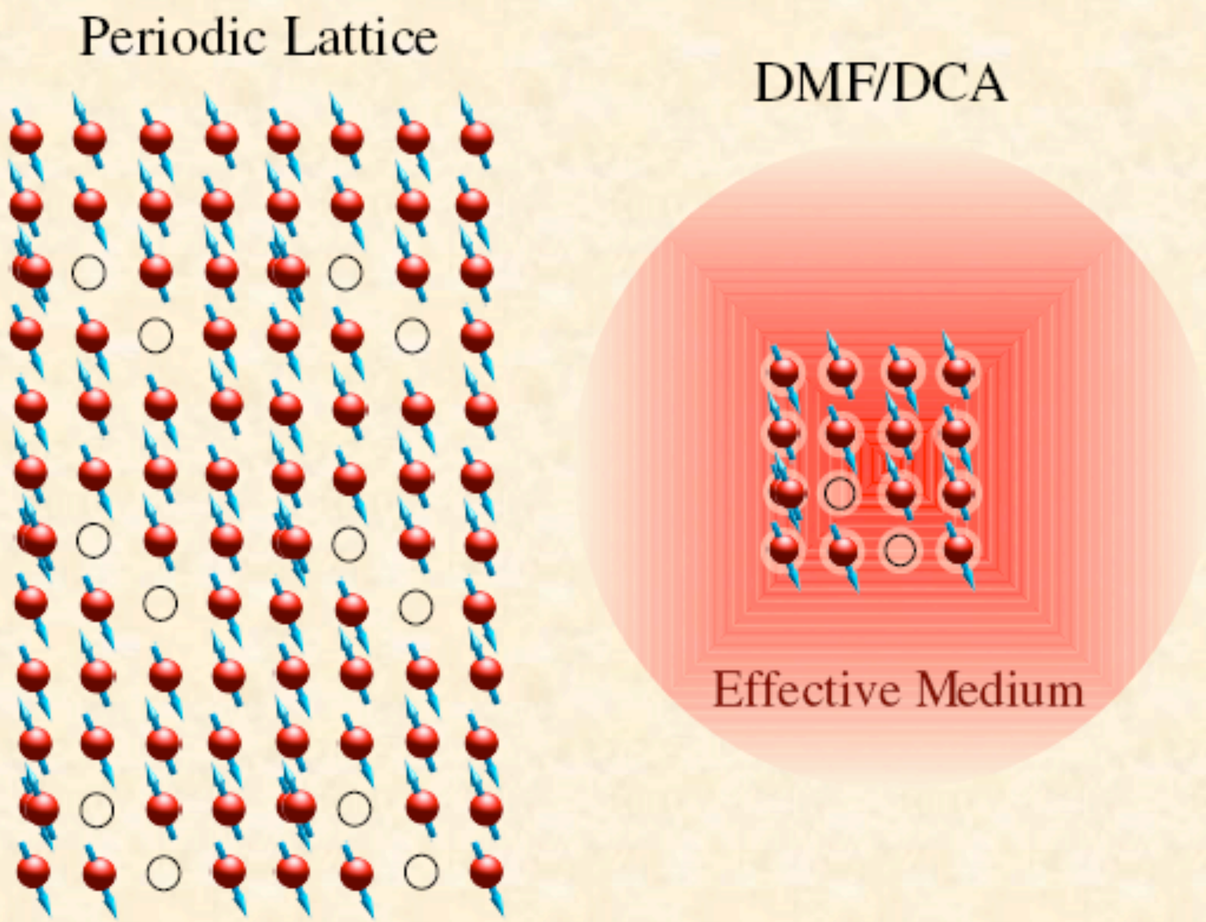
Complexity at the nanoscale

- Complex phase diagrams and new states of matter: e.g. Cuprates, manganites, ruthenates, DMSs…
- Proper understanding require simulations at long length scales



E. Dagotto, Complexity in Strongly Correlated Electron Systems, Science, **309**, 257 (2005)

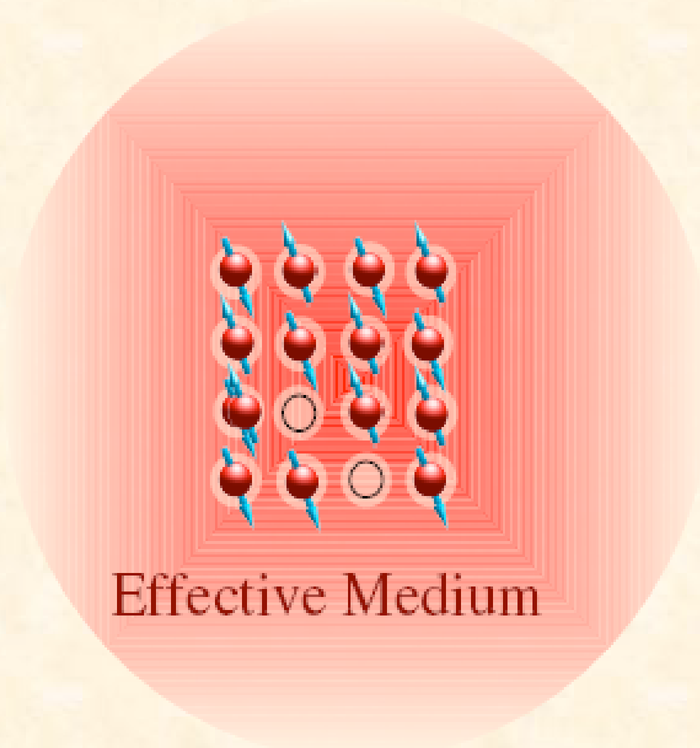
Present Approach



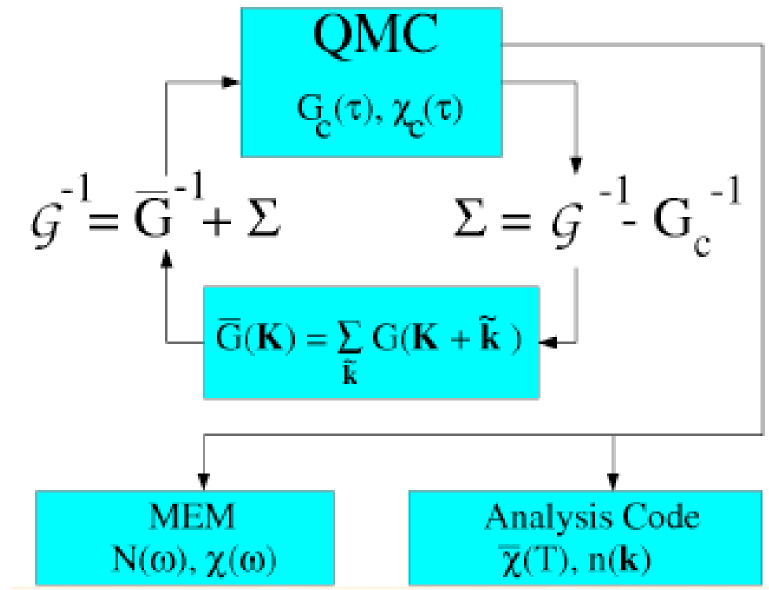
- **A multi-scale approach**
- **Short length scales, within the cluster, treated explicitly.**
- **Long length scales treated within a mean field.**

For a review of quantum cluster approaches: Th. Maier *et al.*, *Rev. Mod. Phys. 77, pp. 1027 (2005).*

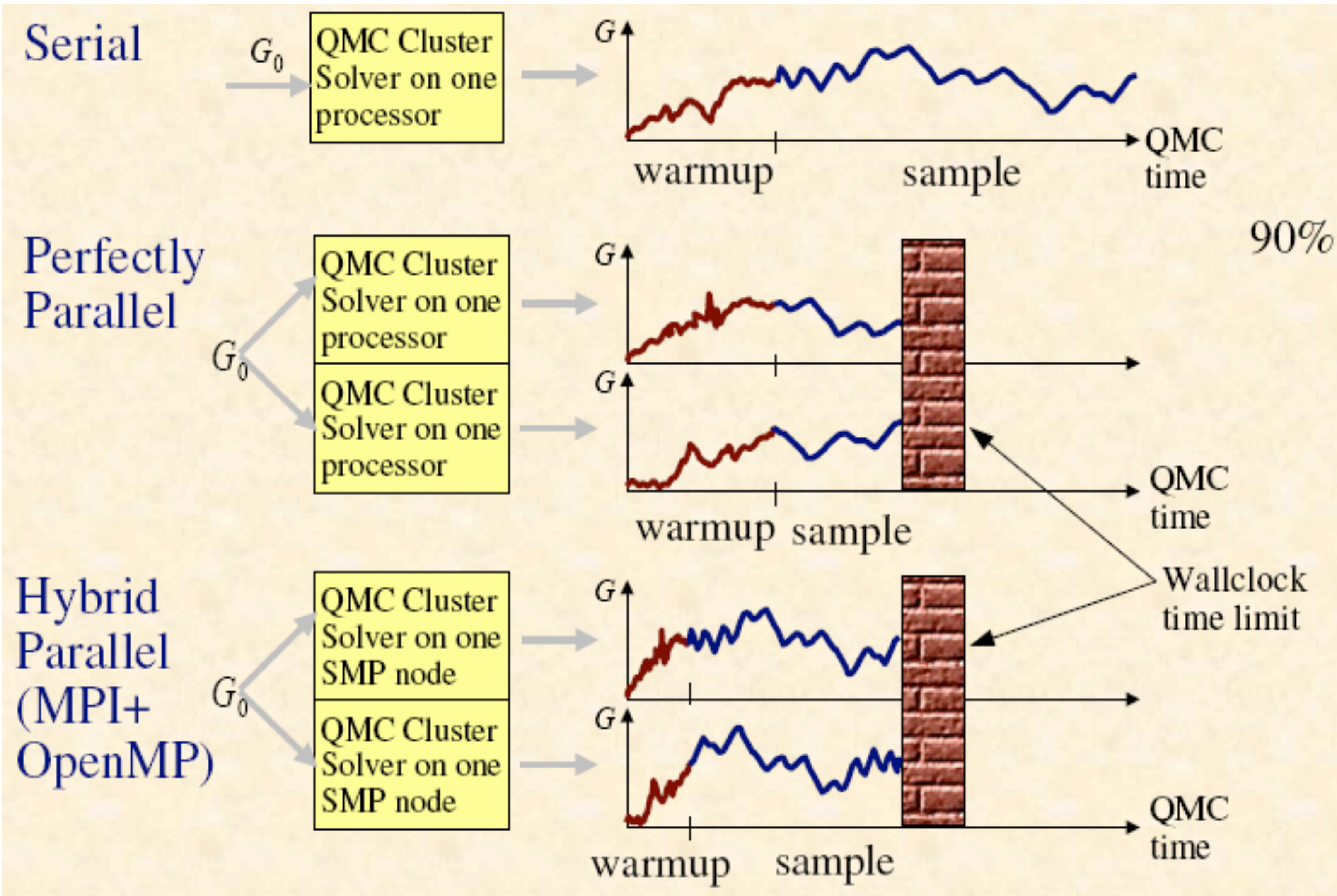
QMC Cluster Solver



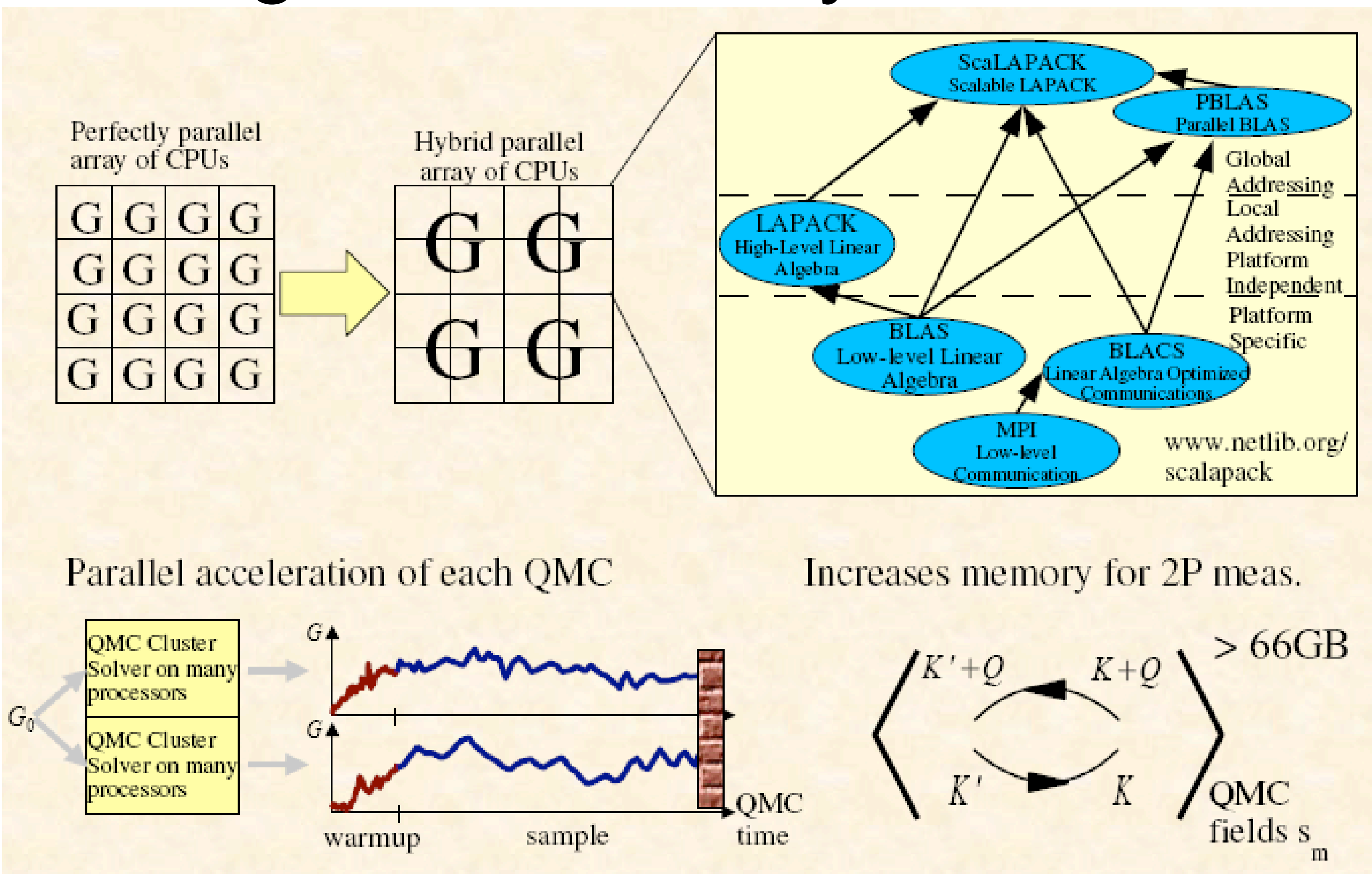
- QMC in the Infinite Dimensional Limit, M. Jarrell, QMC Methods in CM Physics, Ed. M. Suzuki, (World Scientific, 1993), p221-34.
- The Hubbard Model in Infinite Dimensions: A QMC Study, Mark Jarrell, Phys. Rev. Lett. 69, 168-71 (July 1992).
- A QMC Algorithm for Non-local Corrections to the Dynamical Mean-Field Approximation, M. Jarrell, PRB 64, 195130/1-23 (2001).



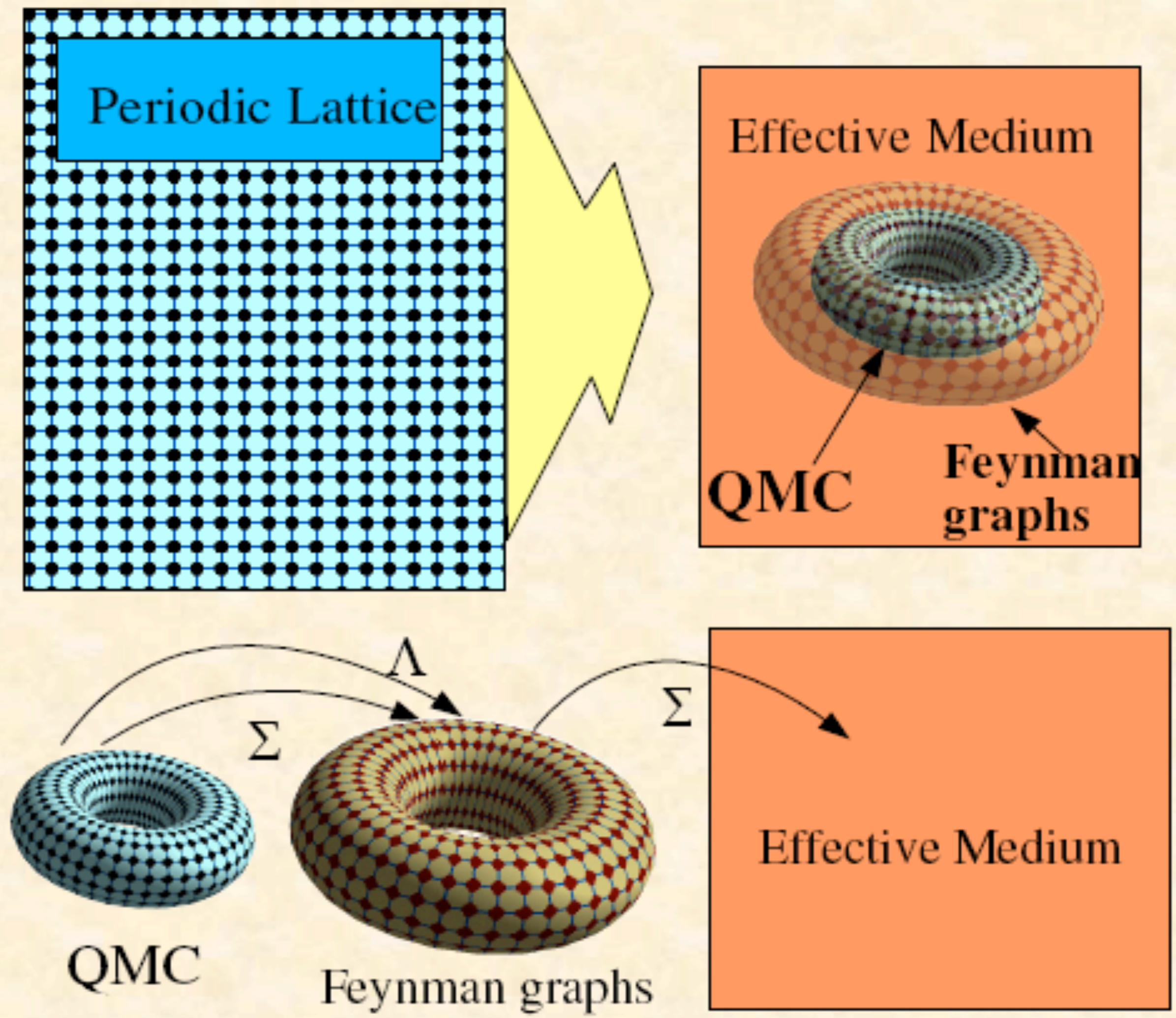
Parallelization of the QMC solver



Improved QMC solvers at short length scales – Hybrid QMC

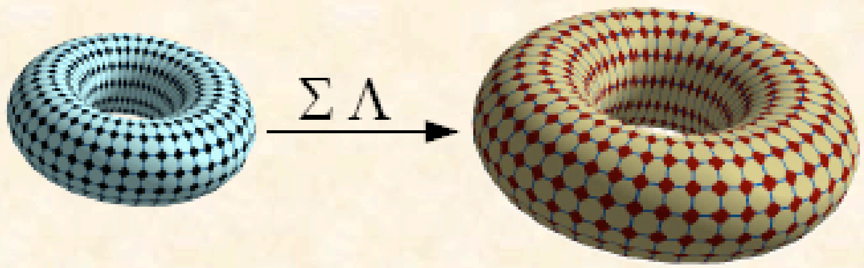


Multi-scale Many-Body formalism



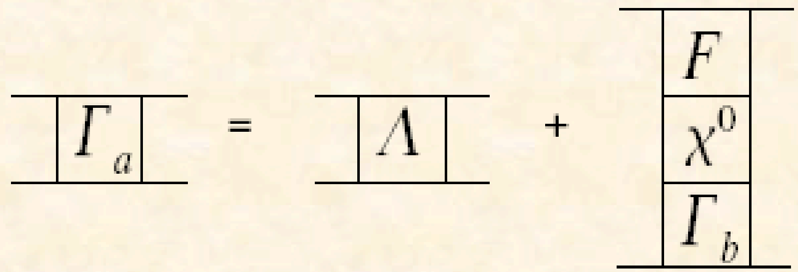
- Appropriate method for each length scale
  - short = explicit
  - intermediate = perturbative
  - long = mean field
- Only MB processes from explicit calculation
  - Σ and Λ from QMC input to diagrammatic caclulation

Intermediate length scale – Diagrammatic Approach

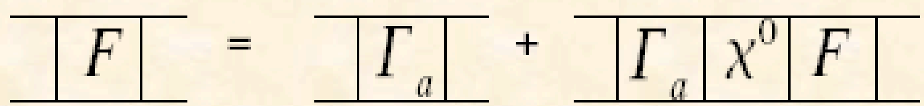


- Large cluster: solve parquet and Bethe-Salpeter equations self consistently.
- Σ, Λ from QMC
- Γ, F, χ size nt >1600
- distribute data on Q

Parquet e.q. $\Gamma_a(K,K',Q)=\Lambda(K,K',Q)+(\Gamma_b\chi^0F)(-K',-K,K+K'+Q)$



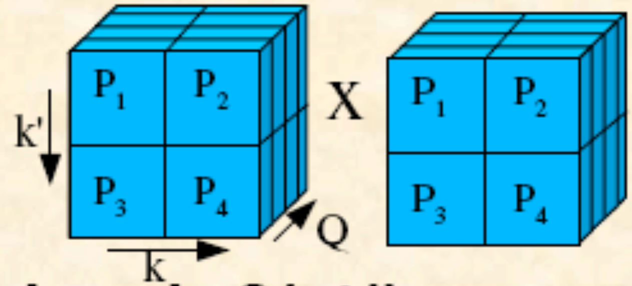
Bethe-Salpeter e.q. $F(K,K',Q)=\Gamma_a(K,K',Q)+(F\chi^0\Gamma_a)(K,K',Q)$



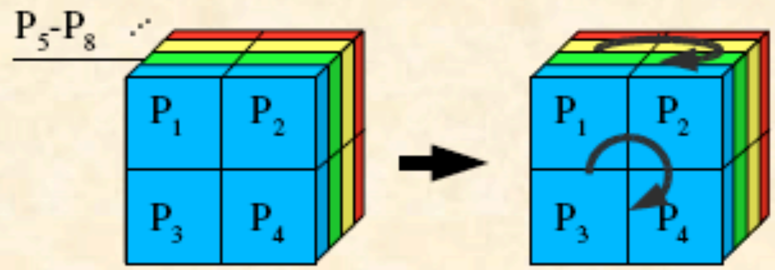
N. Bickers
D. Hess
V. Janis

Major Performance Bottlenecks

- Computational Bottleneck
  - Bethe-Salpeter Equation:



    - like 3D Matrix Multiplication
      - $O(nt^4)$ operations, so main loop is $O(nt^4)$
    - Dramatically limits size of computation
- Communication Bottleneck

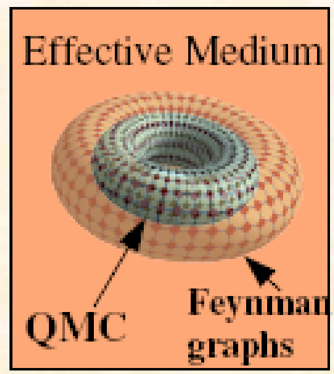


  - Parquet Equations
    - Rotation of matrices:
      - Complex and Global message transferring pattern
      - Each Parquet Equation: $O(nt^3)$ messages
- Both are recalculated on each iteration
- No Minus sign problem
  - Algebraic rather than exponential scaling!

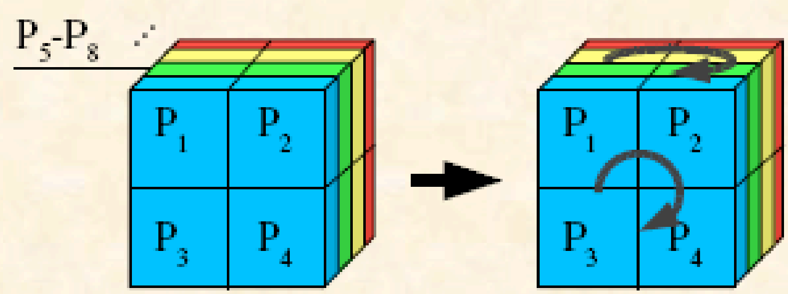
doable.

Summary

- Present methods cannot address multi-scale phenomena displayed by correlated materials
  - Minus sign problem
  - Complexity (number of correlated orbitals)
- MSMB method treats each length scale with an appropriate method
  - short = explicit
  - intermediate = diagrammatic
  - long = mean field



- Challenges, Outreach, Collaboration
  - MP QMC for measurements of Γ, F, etc.
  - Large matrix (tensor) algebra
  - Web distribution of codes (9/07)



http://scicompforge.org/petamat