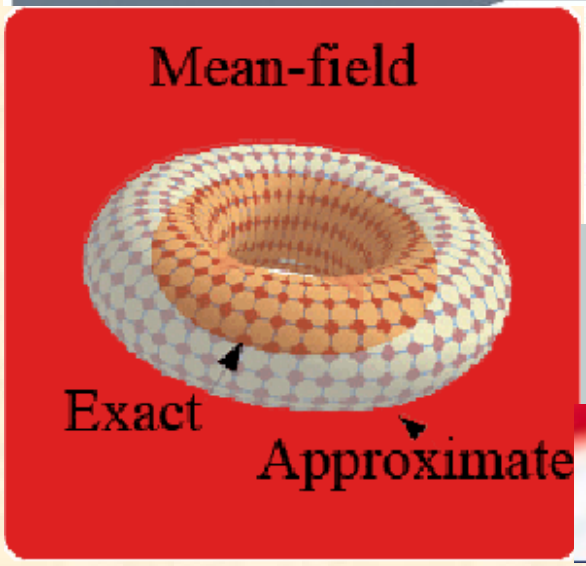
Massively Parallel and Multi-Scale Simulations of Strongly Correlated Materials

LONI, Oct. 30, 2008, Baton Rouge

SciDAC
Scientific Discovery through Advanced Computing



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Outline

- Introduction
  - The MS challenge to MBT
  - Present Approach
- MSMB Approach
  - Separation of length Scales
  - Diagrammatic methods at long length scales
  - Improved Cluster Solvers at short lengths
  - Integration of approaches and with LDA
- Outlook and Outreach

Outline

- **Introduction**
  - **The MS challenge to MBT: complexity**
  - **Present Approach**
- **MSMB Approach**
  - **Separation of length Scales**
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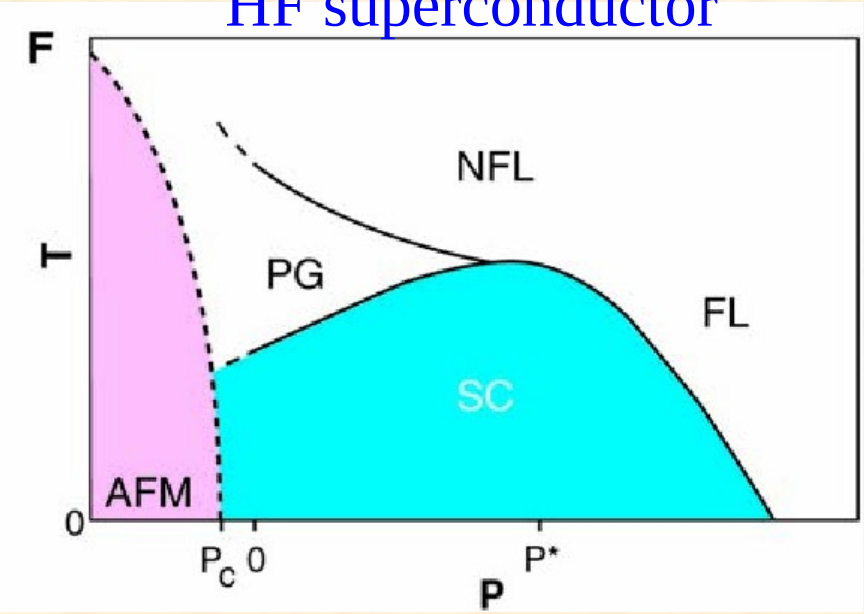
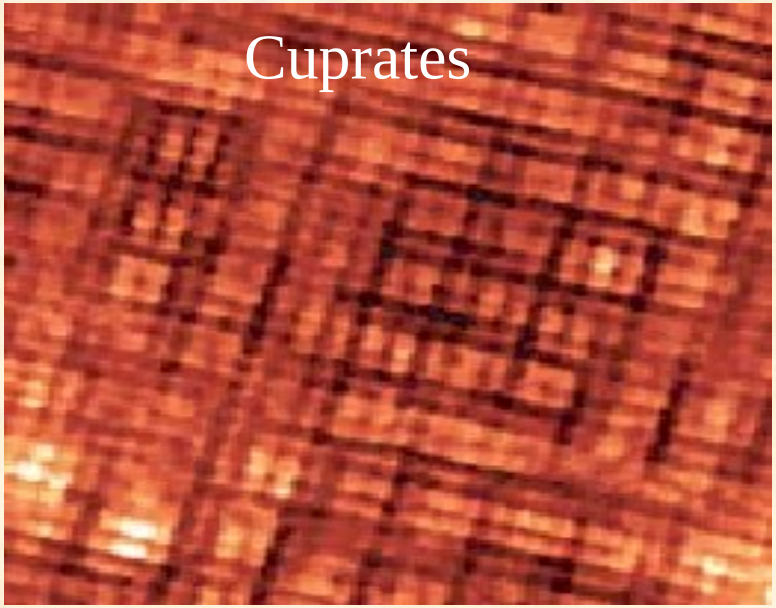
Complexity: the challenge to MBT

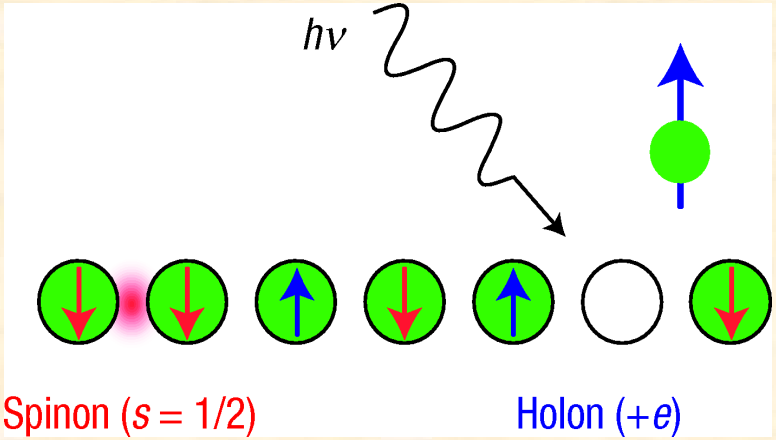
HF superconductor



Cuprates

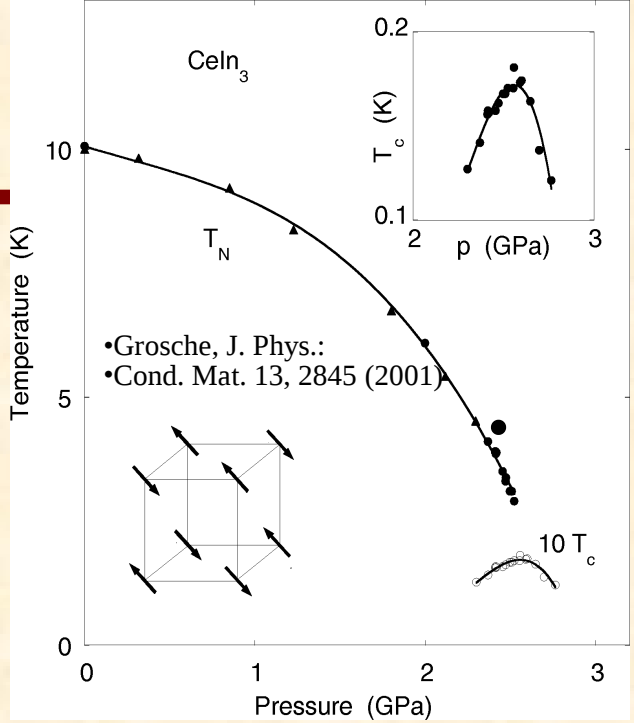


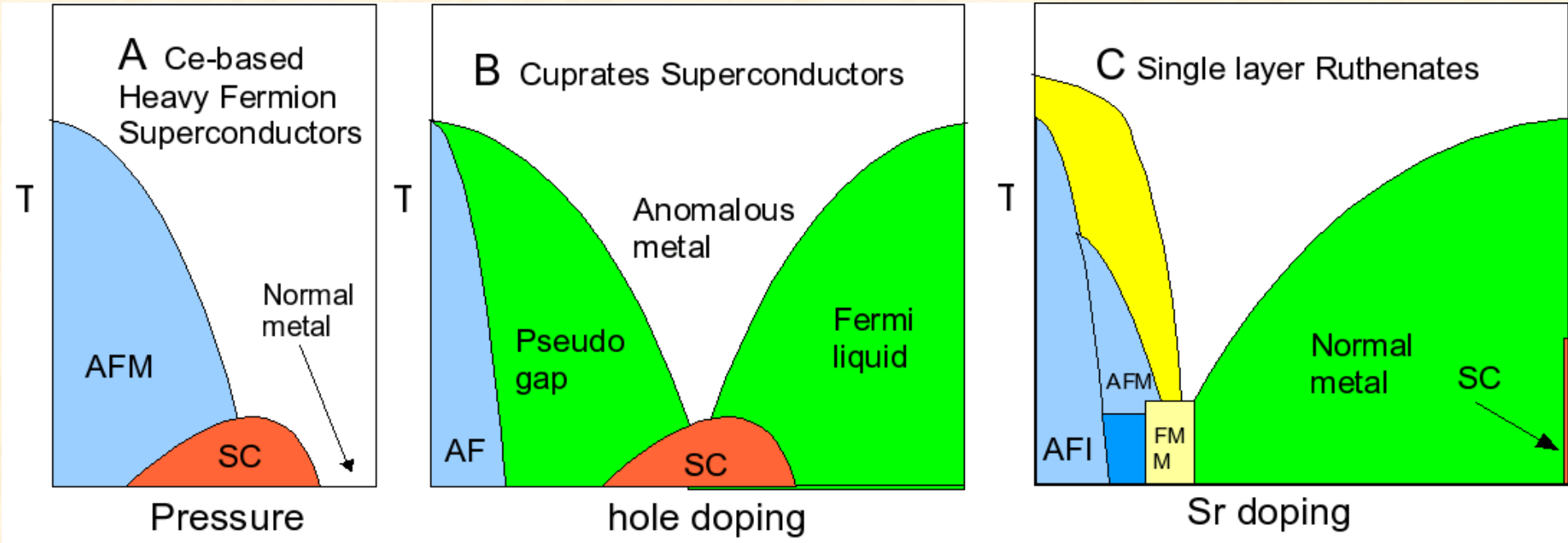
- **Complex phase diagrams**
- **Complex Spin and charge ordering**
- **Complex excitations**



Complex Phase Diagrams

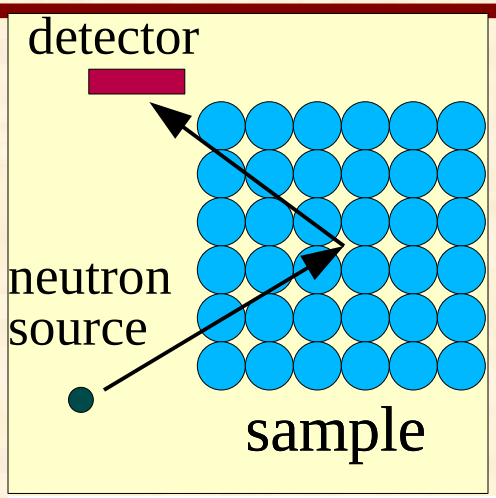
- Competing Ground states
  - E.g. Fermi liquid vs. AFM in CeIn3
  - Complexity at crossover
- Far more complexity in Cuprates, Ruthenates, Manganites, etc.
- Requires long length scales (why?)



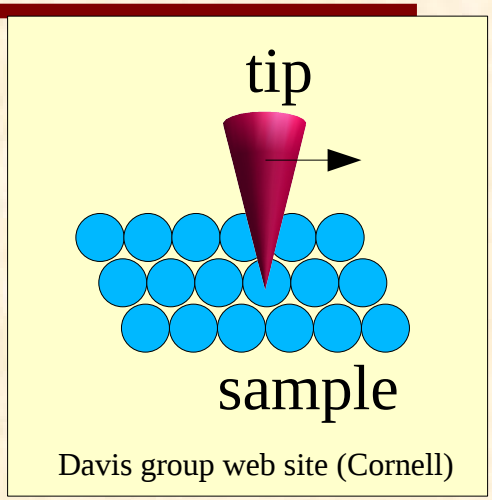


E. Dagotto, Complexity in Strongly Correlated Electronic Systems, Science, 309, p257-262 (2005).

Complex Spin and Charge Ordering

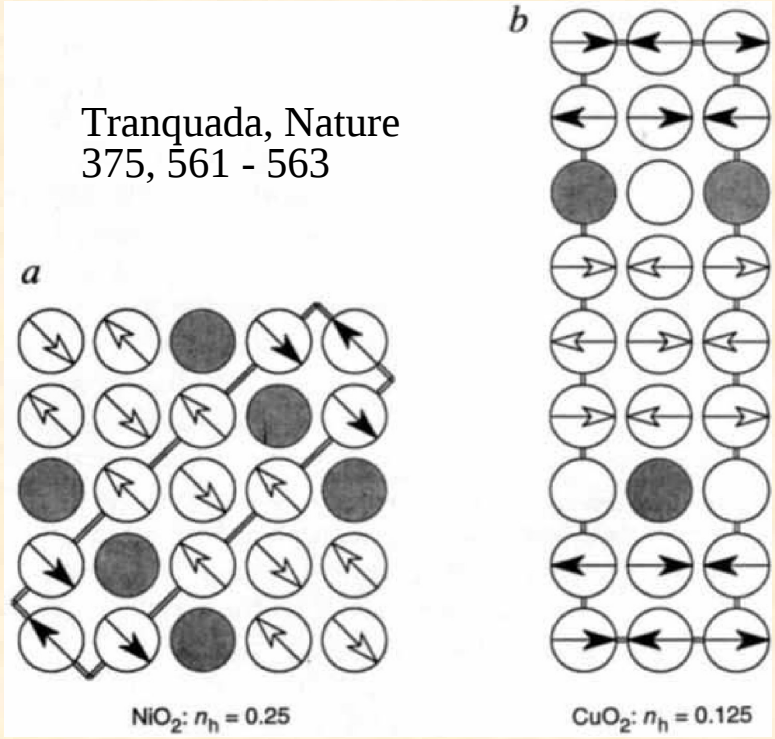


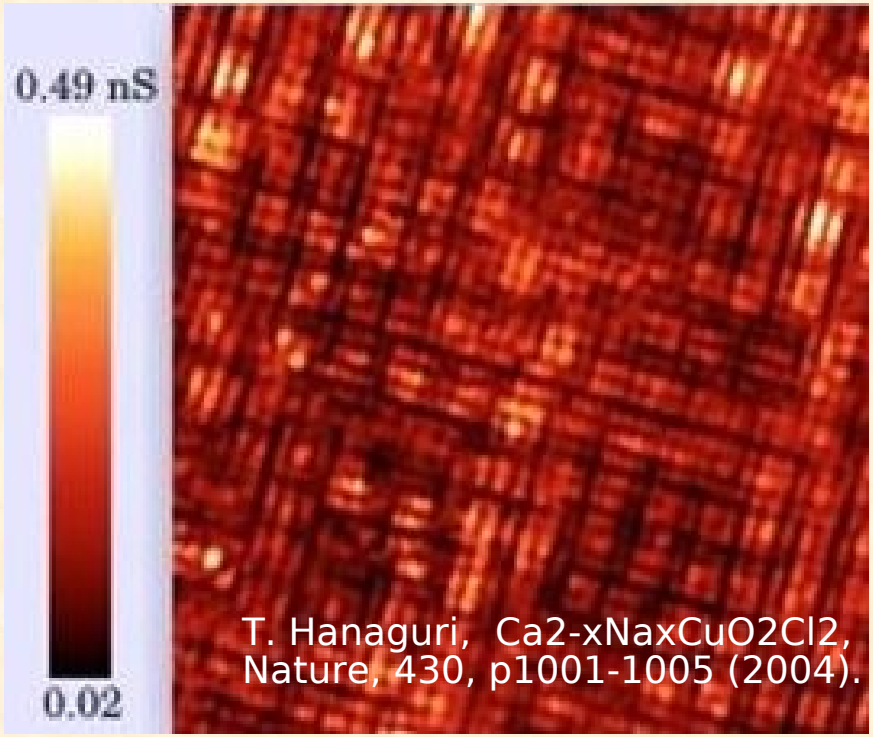
- Spin and charge ordering
  - neutrons, STM, etc.
  - Incipient phase separation
- Seen in other systems
  - CT salts
  - actinides



Davis group web site (Cornell)

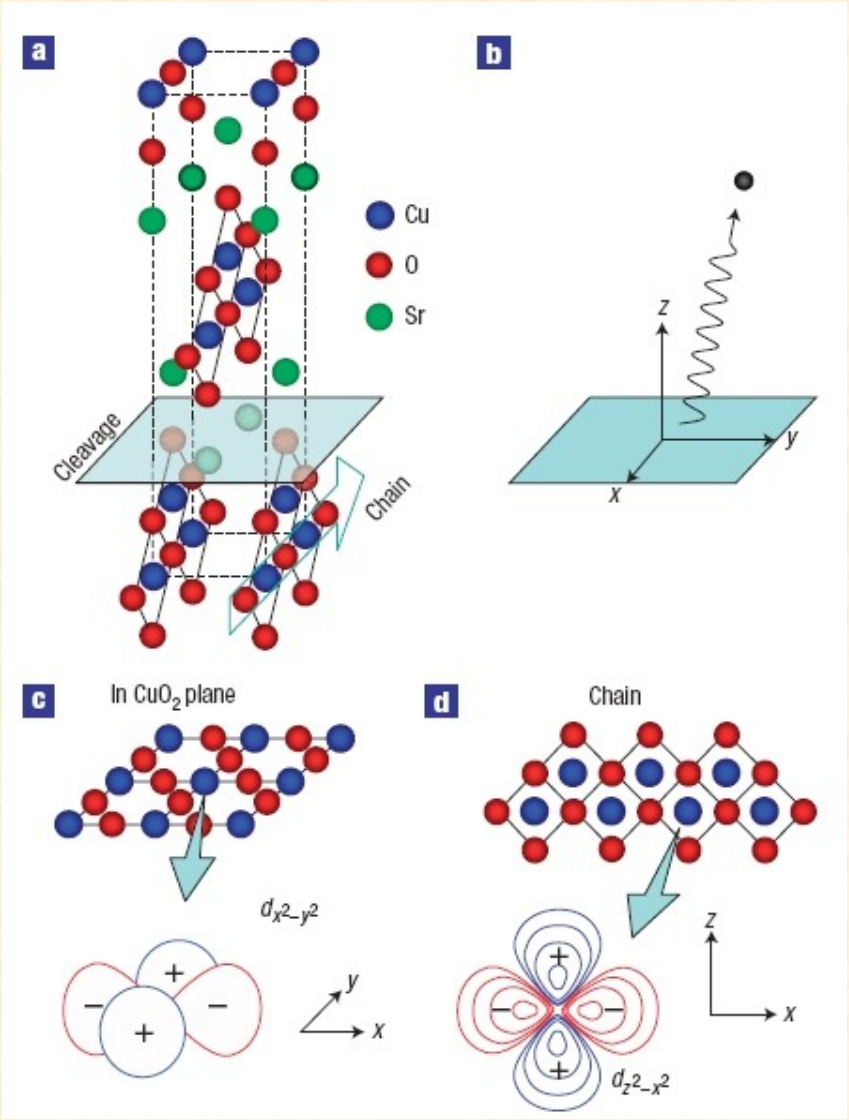
Tranquada, Nature 375, 561 - 563

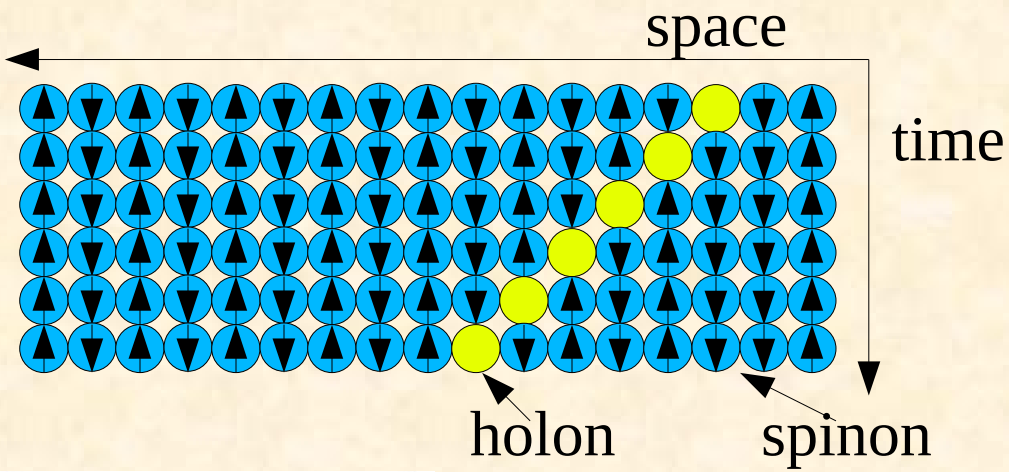


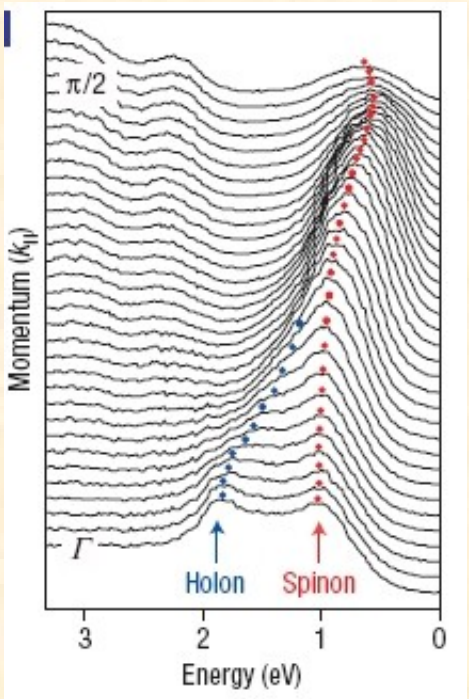


T. Hanaguri, Ca2-xNaxCuO2Cl2, Nature, 430, p1001-1005 (2004).

Complex Elementary Excitations







- Spin-charge separation seen in $SrCuO_2$, Kim, N. Phys 2006
- Complex excitations in other materials

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- **MSMB Approach**
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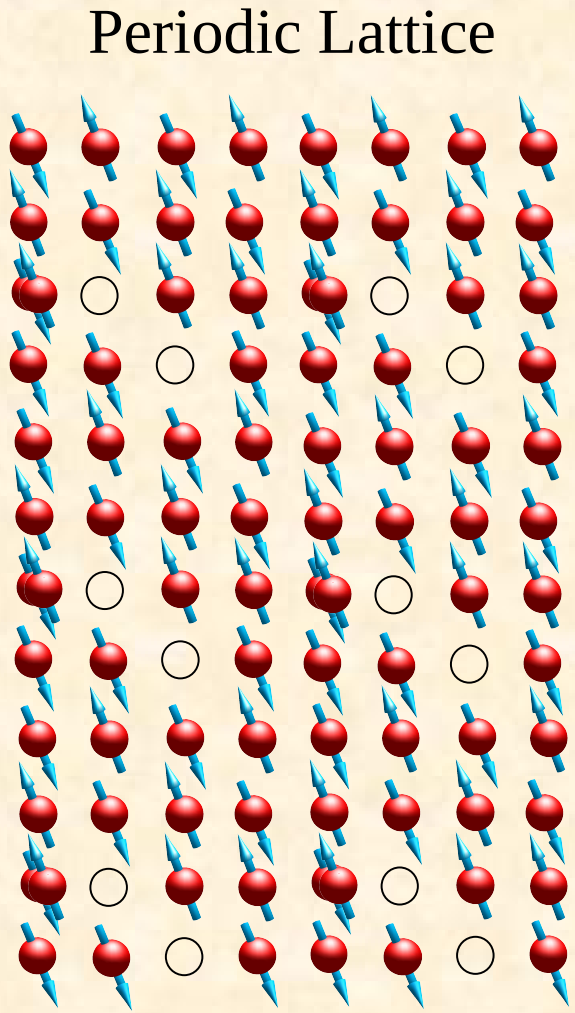
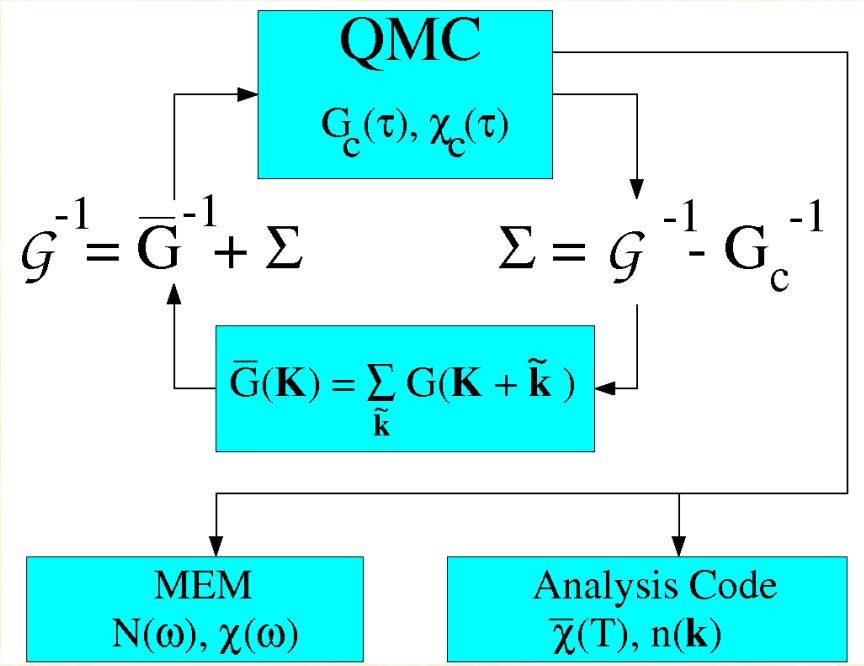
Present Approach



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

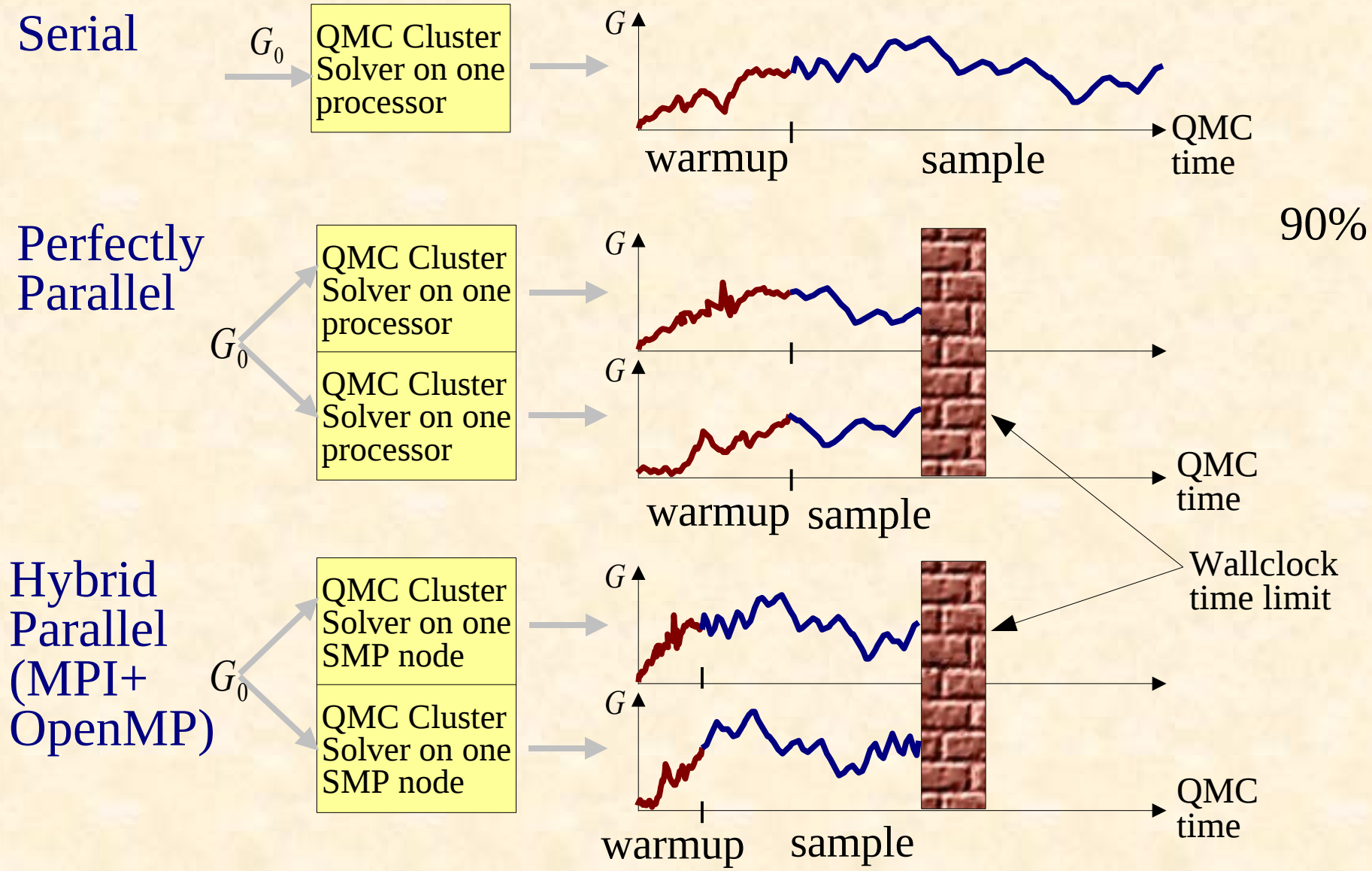
For a review of quantum cluster approaches: Th. Maier *et al., Rev. Mod. Phys. 77, pp. 1027 (2005).*

Quantum Monte Carlo (QMC) Cluster Solver

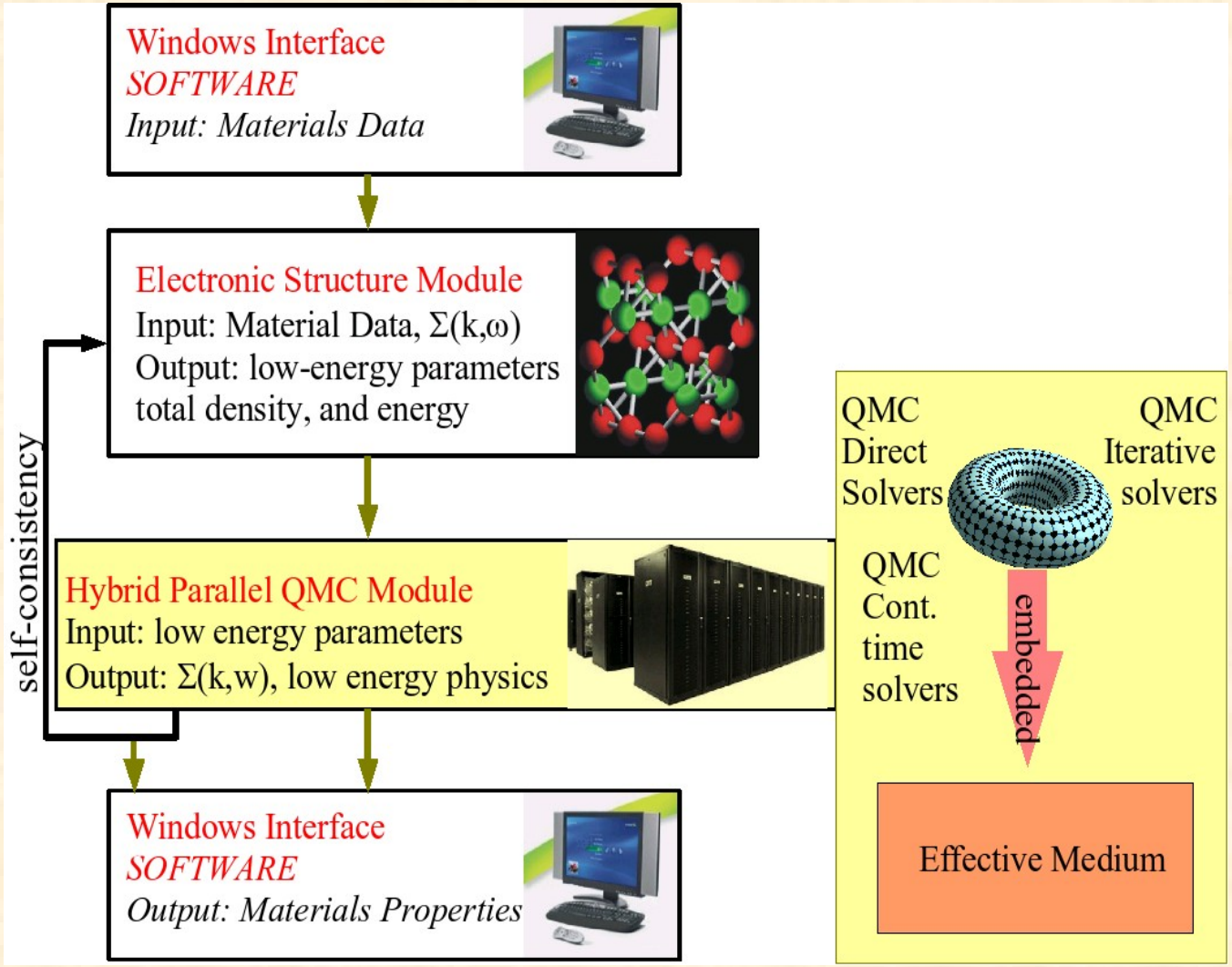


•QMC in the Infinite Dimensional Limit, M. Jarrell, QMC Methods in
•CM Physics, Ed. M. Suzuki, (World Scientific, 1993), p221-34.
•The Hubbard Model in Infinite Dimensions: A QMC Study,
•Mark Jarrell, Phys. Rev. Lett. 69, 168-71 (July 1992).
•A QMC Algorithm for Non-local Corrections to the Dynamical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

Parallelization of QMC Cluster Solver



Integration with LDA and GUI



- LDA is combined with DMF/DCA and other Quantum cluster methods
- First principles including correlation effects
- GUI for acc. to non-experts
- Our approach employs a self-energy based LDA

S. Savrasov recent RMP

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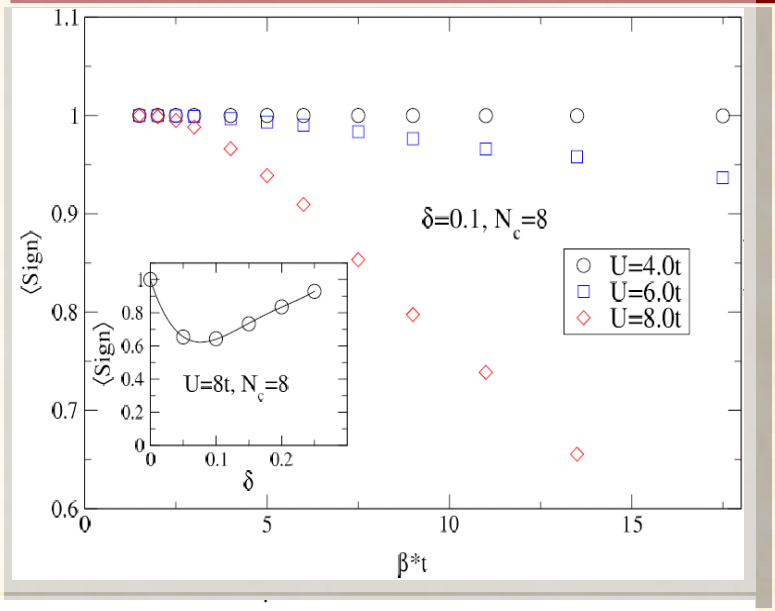
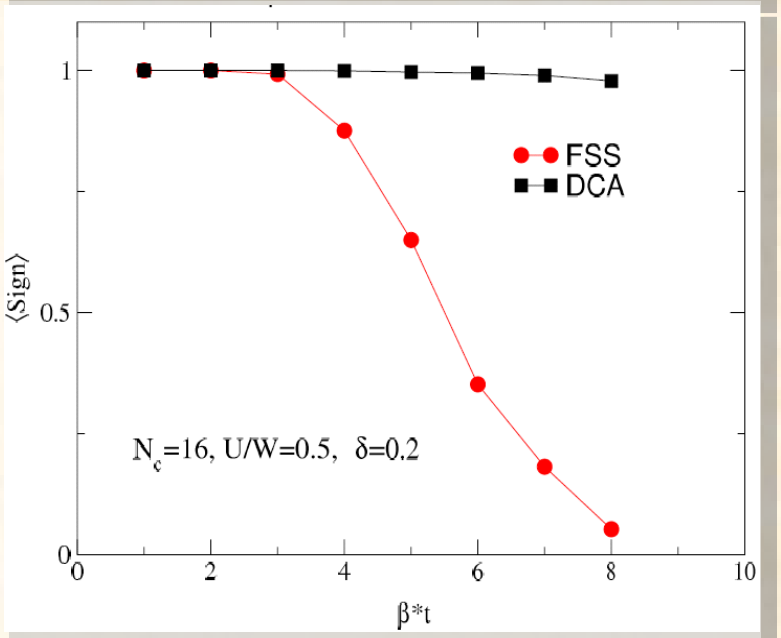
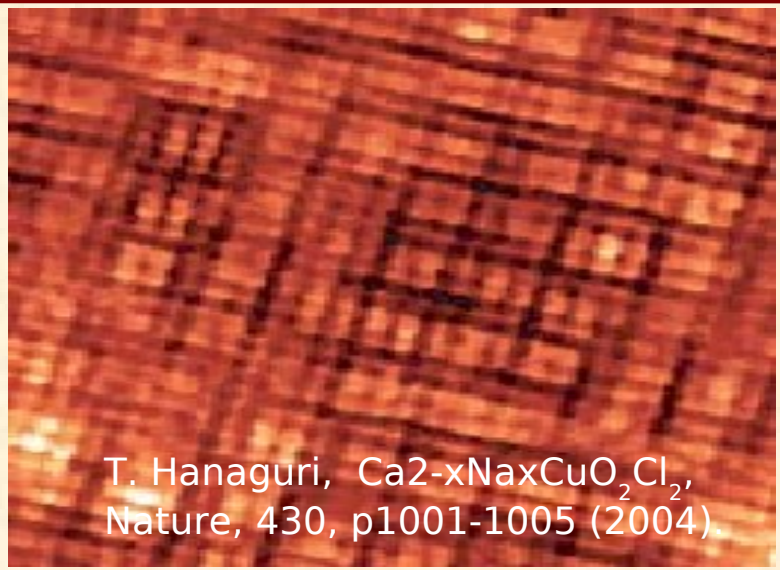
Challenge: QMC sign problem







- **Repeat length of spin and charge ordering many lattice spacings.**
- **Sign problem $\langle m \rangle = \langle mS \rangle / \langle S \rangle$.**
- **Prevents us from treating these correlations explicitly.**
- **Sign problem is NP hard (M. Troyer, PRL 94, (2005)), $\langle S \rangle$ is big only by accident.**
- **More computing helps, but ... better algorithms are needed for long lengths!**

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- **MSMB Approach (Transformative Potential)**
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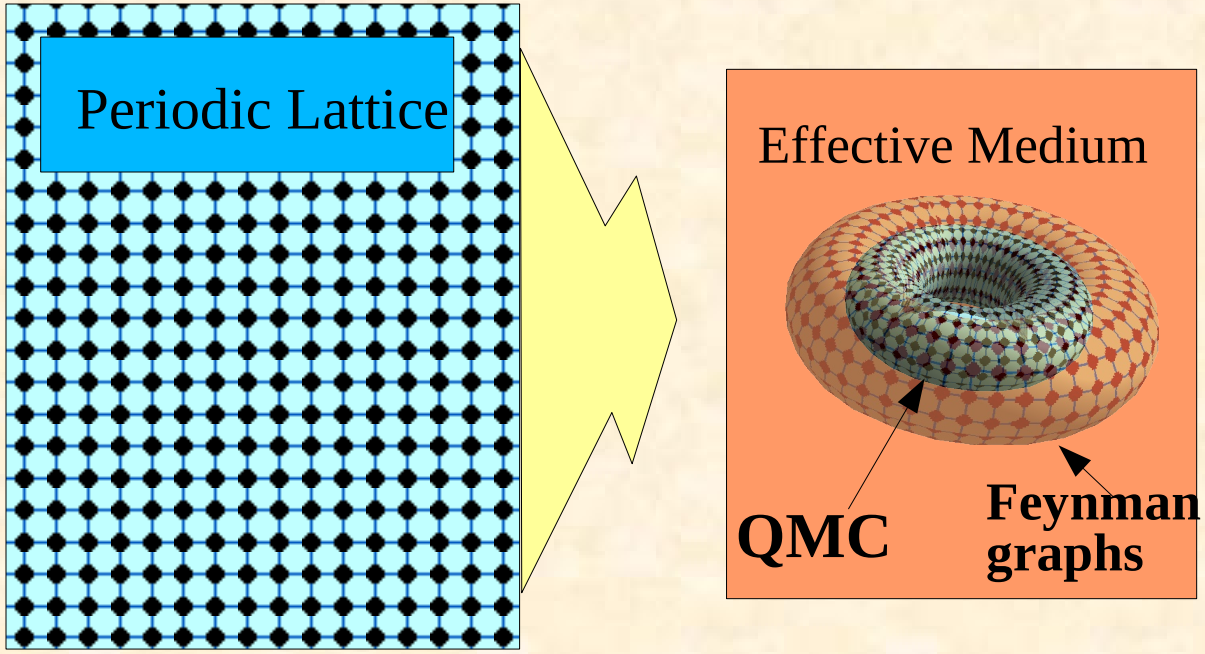
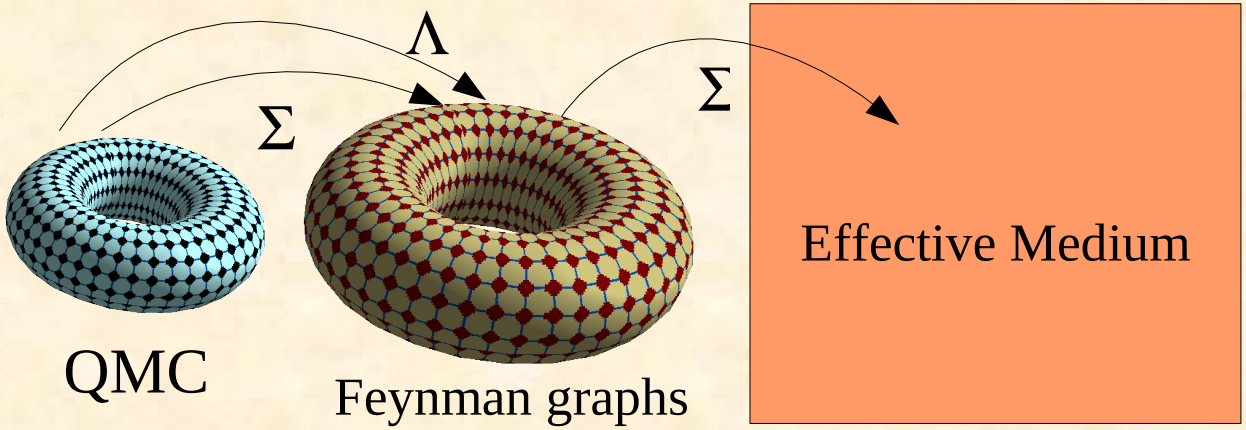
Introduce and Additional Length Scale





- **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**

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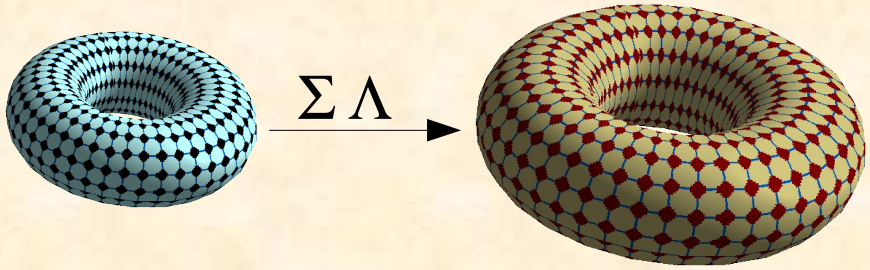
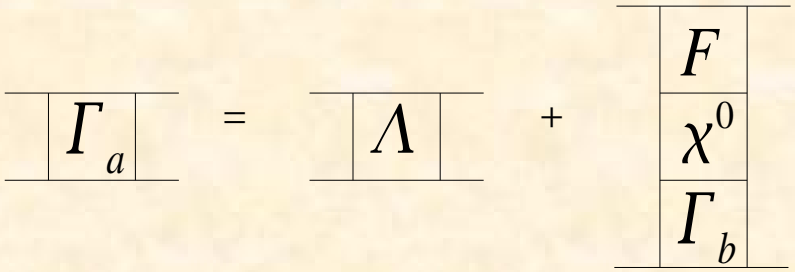
Diagrammatic Methods (Feynman Graphs)

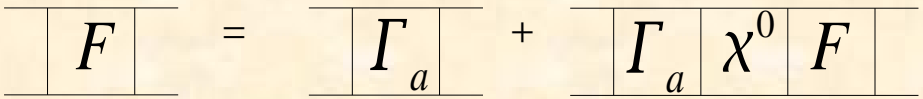


•Large cluster: solve parquet and Bethe-Salpeter equations self consistently.
•Σ, Λ from QMC
•Γ, F, χ size nt >1600
•distribute data on Q

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



- **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
many others

bottlenecks...

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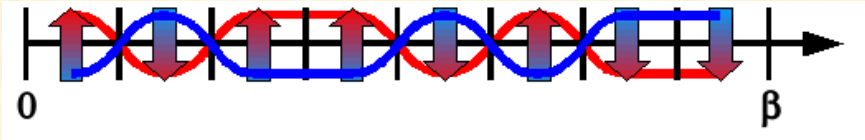
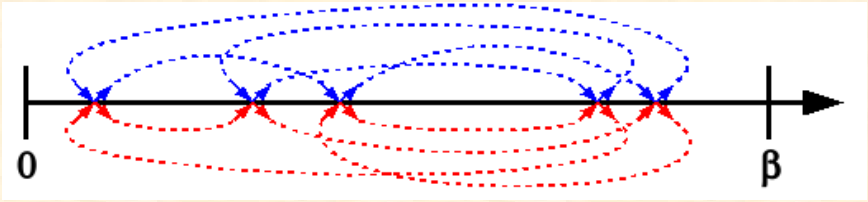
New QMC methods

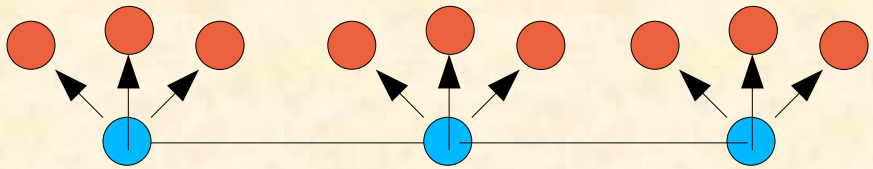
Hirsch-Fye QMC
- discretization in imaginary time
- sampling over field configurations
- systematic error due to discretization
- Hybrid Parallel (Scalapack)



- Continuous time QMC
- variable number of interaction vertices
- sampling vertex configurations
- no systematic errors
- highly anisotropic systems

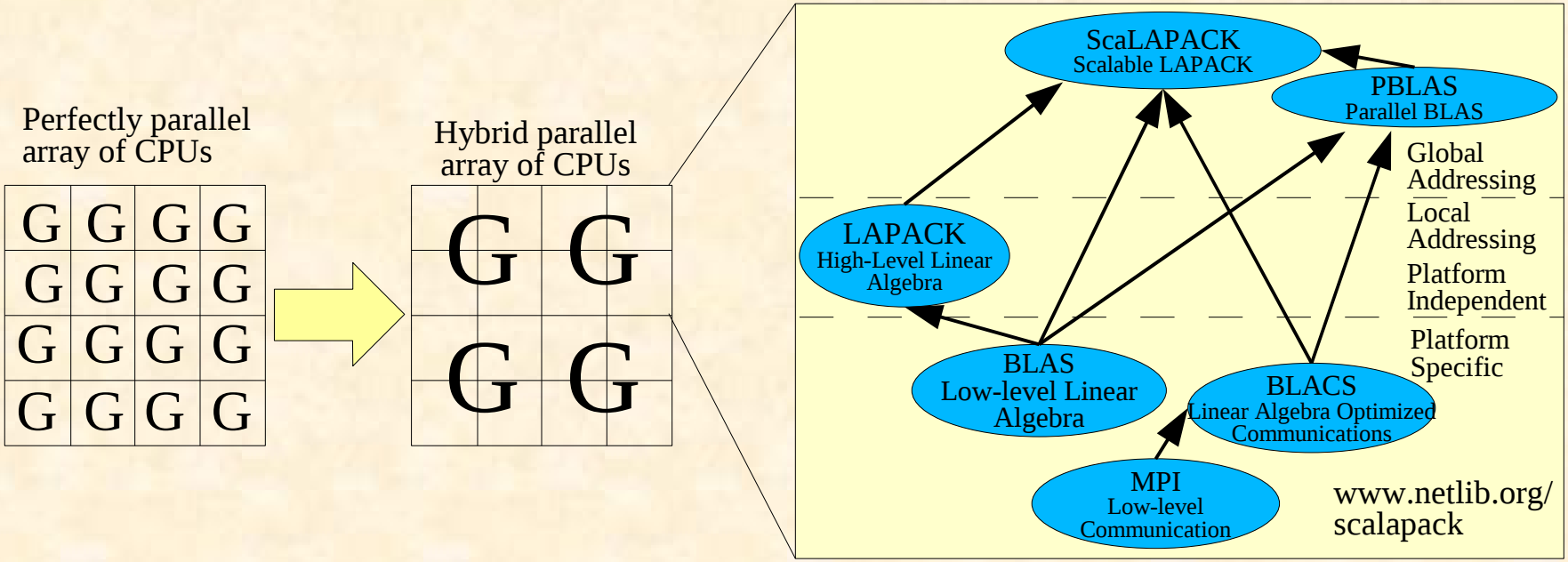


- Linear In β QMC
- variation of DQMC
- add bands to emulate host

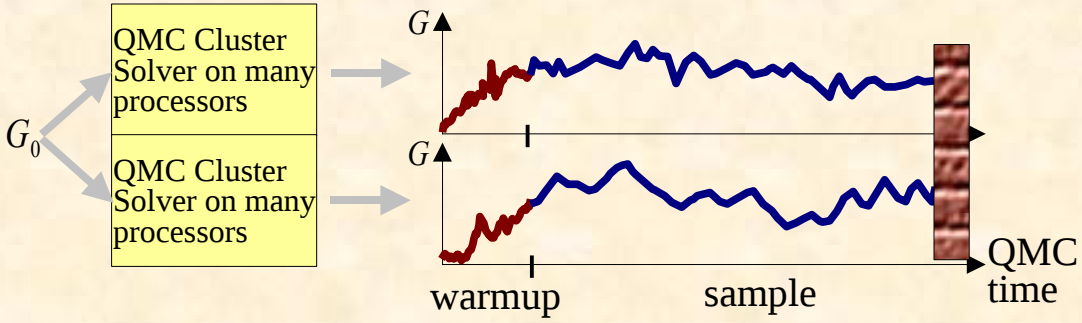


Hirsch, PRL, 56, 2521, (1986)
Rubtsov, PRB, 72, 035122, (2005)

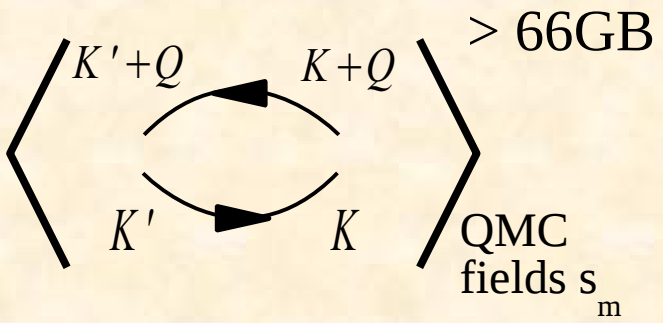
Hybrid Parallel QMC



Parallel acceleration of each QMC



Increases memory for 2P meas.



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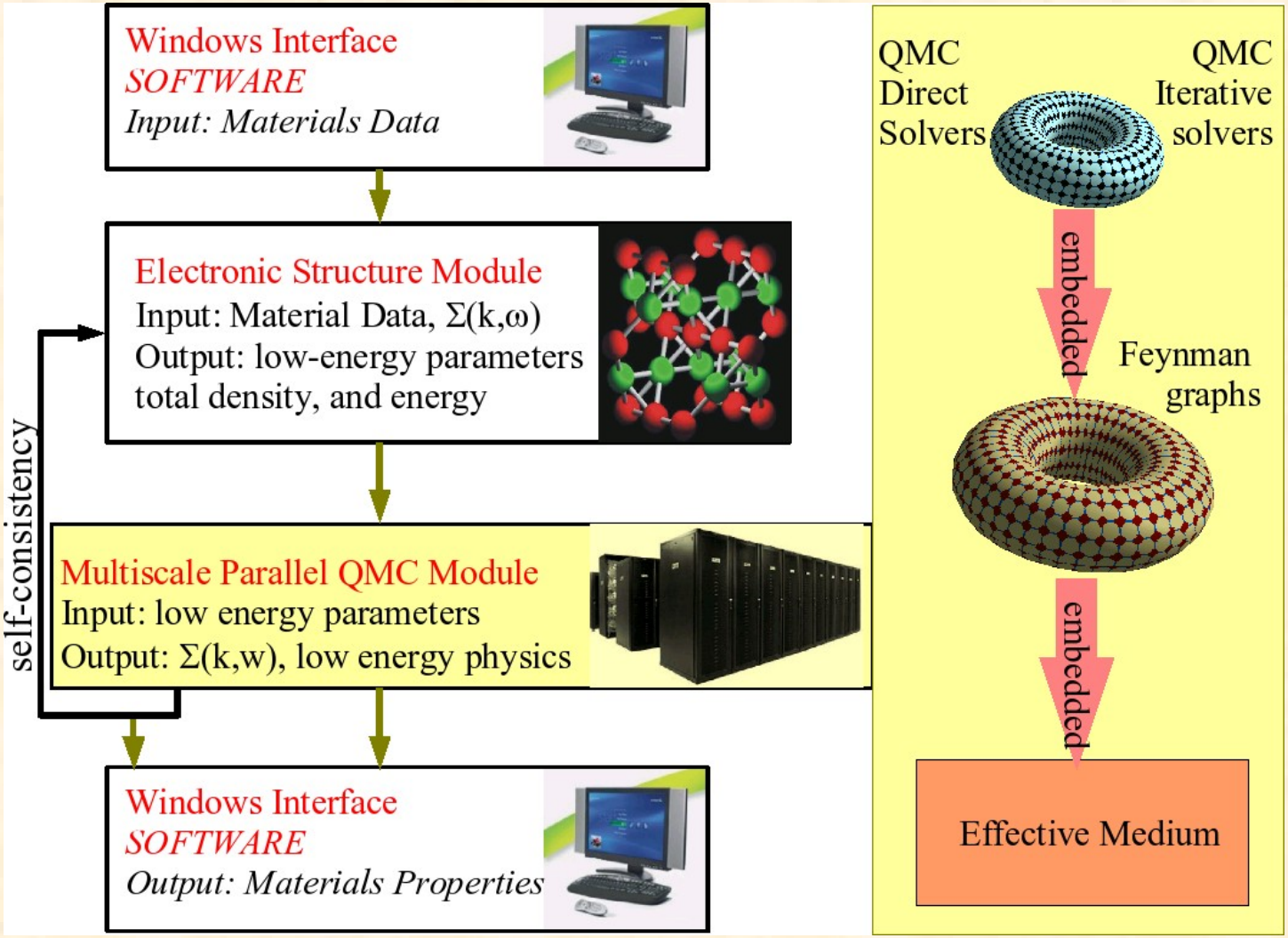
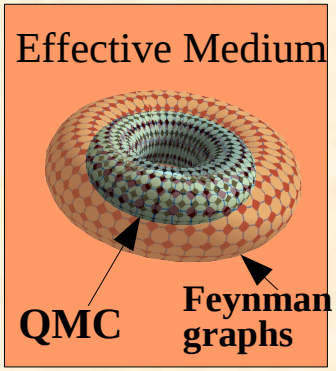


- LDA is part of MSMB approach
- First principles including correlation effects
- Our approach employs a self-energy based LDA
- More than just MSMB replacing DCA or DMF...

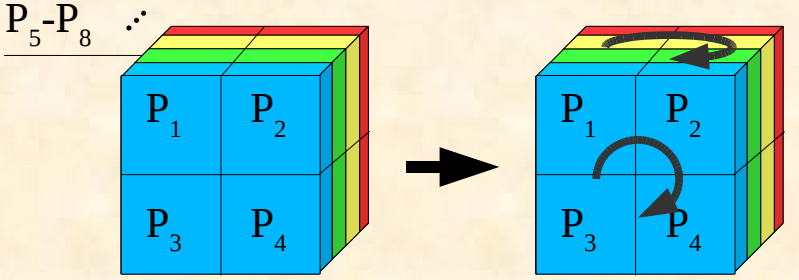
Outlook and Outreach

- **Present methods cannot address multi-scale phenomena**
  - **Minus sign problem**
  - **Complexity (number of correlated orbitals)**
- **MSMB 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**
  - **MP Non-linear systems**
  - **Heterogeneous computing**
  - **Education!**



$$\Gamma_a = \Lambda + F\,\chi^0\,\Gamma_b$$

$$F = \Gamma_a + \Gamma_a\,\chi^0\,F$$



http://scicompforge.org/petamat
http://www.pirealps.org

Graduate Education

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  - Programming Techniques for Physics Simulations
  - Computational Physics (MT)
  - Computational Science (KT)
  - Comp. Methods and Alg. in Many-body Theory (TP)
- Students spend 1 year abroad
- EU students visit US partners
- Scientific C++, CSci, Elem. SS.