

# Computational Physics @ HRI

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# Outline of the talk

- Computational Cosmology
- First Principle Calculation
- Correlated Electron Systems

## Computational Cosmology: Numerical Simulations of gravitational clustering and galaxy formation.

- **Simulations:** These are simulations using interacting particles with the primary interaction being gravitational. We have run simulations with up to  $10^8$  particles which requires around  $5 \times 10^{17}$  floating point operations, hence a Teraflop machine can be kept busy for nearly a week.
- **Analysis:** Analysis of each output of an N-Body simulation with  $10^8$  particles required about  $10^{16}$  floating point operations. Observational data sets with a million or more galaxies also require considerable computing power for analysis.
- **Parameter estimation :** Once the observations have been analysed and characterised by a few functions, the next step is to constrain cosmological models. Most cosmological models are described by about 6 – 8 parameters and one must do a

likelihood analysis in this parameter space. The task is more complex than finding the best fit model as one must find all models allowed by observations with a given probability. Parameter estimation for a model with 6 parameters takes about  $10^{15}$  floating point operations.

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<sup>a</sup>J. S. Bagla, H. K. Jassal, Nishikanta Khandai

**First Principle Calculation:** Density functional theory methods using both plane wave basis sets and atom-centered local basis sets. Wave function based methods: HF and quantum Monte carlo being studied.

- Electronic, magnetic and structural properties of atomic clusters and mixed-metallic clusters. Particularly, TM-doped alkali metal clusters.
- Exploring nanostructured materials as possible hydrogen storage medium.

For these, available DFT and quantum chemistry packages will be used. Developing applications. Finding lowest-energy structures of atomic clusters is a challenging optimization problem. We plan to develop codes based on various global search techniques to address these problems. <sup>b</sup>

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<sup>b</sup>Prasenjit Sen, Kalpataru Pradhan

# Correlated Electron Systems

- Disordered electrons strongly coupled to classical fields: The outstanding problems in this field relate to transition metal oxides, particularly the manganites. Computational Calculation involves Exact Diagonalisation.
- Cellular dynamical mean field theory (C-DMFT) for fermions: Dynamical mean field theory has become a standard, almost indispensable, many body technique today. The original single site approximation, exact in “infinite dimensions” has now been extended to finite dimensions by embedding finite clusters in a specific low dimensional bath.
- Fluctuation exchange/Eliashberg schemes for superconductivity: Interacting electron problems can sometimes be handled through self consistent approximations for the single particle Greens function,  $G_{\mathbf{k}}(\omega)$ , and the

self-energy,  $\Sigma_{\mathbf{k}}(\omega)$ . Combining the strong correlation solution from DMFT with a Eliashberg like approximation (in 3D) to study broken symmetry phases, magnetism and superconductivity, in heavy fermion systems. The computational effort involves solving a nonlinear integral equation in  $3 + 1$  dimension, discretising the momentum and frequency variables.

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<sup>c</sup>Pinaki Majumdar, Kalpataru Pradhan, Anamitra Mukherjee, Vivekanand singh