

# HPC to GRID computing at JNU

## Case studies of Life Sciences Applications

Workshop on Developing Applications on Grid - GARUDA

National Grid Computing Initiative - GARUDA

Title of Talk

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## HPC at JNU

- **48-processor Opteron Cluster**
- **16-processor Altix 350 SMP**
- **Expansion planned to 256 processor machine, through CDAC Pune**

**Applications largely for Life Sciences – will expand to Scientific Computing and Social Sciences applications.**

## HPC Life Sciences Applications have a wide range

- **Embarrassingly parallel applications like database searches**
  - Made up of repetitive tasks involving string searches between a query string and the database
  - Each task is completed in a short while (microseconds)
  - Speed of iterative searches are improved using methods such as memory mapping
- **Virtual Screening applications:**
  - As above, made up of repetitive tasks involving the docking of a single receptor structure and a database of drug-like molecules
  - Each task in in seconds-minutes
  - Ideal for loosely-coupled architectures – testing heterogenous architecture and OS
- **Molecular simulations which do not normally scale well beyond a few nodes.**

## HPC computing at JNU

- **HPC in JNU has largely been used for Life Sciences Applications**
  - Linear scaling – Database searching
    - MPI based
      - Mpi-BLAST
    - PVM based
      - Hmmer
  - High-Throughput based
    - DOCKING
  - Non-linear scaling: Molecular simulations
    - Molecular Dynamics Scaling
  - Data access
    - Biomirror

# Life Sciences Grid Computing

## Deploy Existing Portals on the Grid

- BRAF from CDAC-Pune

## Commonly used applications

- Linear scaling – Database searching
  - MPI based
    - Mpi-BLAST
  - PVM based
    - Hmmer
- High-Throughput based
  - DOCKING
- Non-linear scaling: Molecular simulations
  - Molecular Dynamics Scaling

## Data

- Bio-Mirror

## In-house applications