

PharmaGrid

**Empowering Pharma Research
Through Cutting Edge Technology**



**National Institute of
Pharmaceutical Education
and Research (S.A.S. Nagar)**

Background

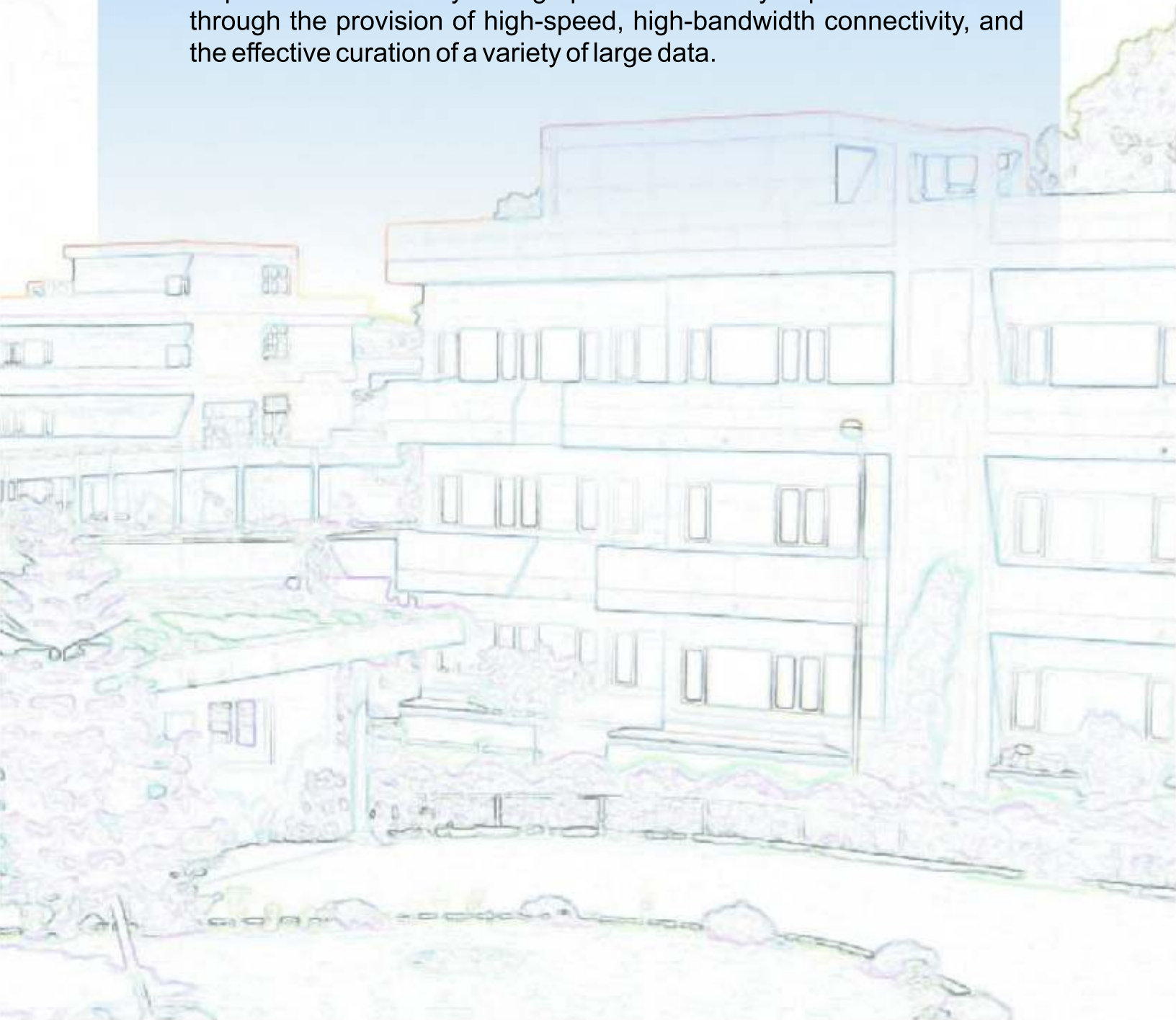
- Grid computing involves the concurrent use of several computers to solve a single problem.
- Participating computers are located over a high speed network (grid) to enable resource sharing to solve large CPU intensive computational efforts.
- Pharmaceutically relevant computational problems are CPU intensive jobs:
 - Molecular dynamics of macromolecules – drug interactions
 - Quantum chemical analysis of drugs
 - Virtual screening of large database of compounds
 - Stepwise understanding of drug metabolism and toxicity processes
 - Atomic level modeling of *in vitro* and *in vivo* processes
 - Integration of atomic level and system level biology
 - Meso scale modeling of drug delivery systems, *and many more*.
- PharmaGrid facility being created at NIPER, S.A.S. Nagar is the central facility to establish a nationwide grid for carrying out pharmaceutical research.



Objectives

The PharmaGrid aims to enhance pharmaceutical research, address grand challenges and grow computational research into a viable mode alongside experiment and theory across all academic disciplines at NIPER.

1. To cater to the needs of pharmaceutical research community with cutting edge technology.
2. To share the computational resources among various NIPERs.
3. To focus on high end computational science, which includes research into mathematical and programming as well as algorithmic development and implementation.
4. To train new generation of computationally skilled researchers in areas underpinned by high end computing, particularly those of important to drug discovery and development.
5. To provide accessibility to large pharmaceutically important databases through the provision of high-speed, high-bandwidth connectivity, and the effective curation of a variety of large data.



Infrastructure

The ability of scientists to perform cutting-edge research and be competitive globally is linked to the availability of state of the art infrastructure. In the field of computational analysis of pharmaceutical samples and processes, high performance computations are essential. The equipment purchased in the first phase of the PharmaGrid project has 3.56 TFlops computational power.



Hardware

Linux Cluster:

200 cores, 1 master node, 24 computation nodes, 20 GBPS speed InfiniBand interconnectivity

Windows Cluster:

72 cores, 1 master node, 8 computation nodes, 20 GBPS speed InfiniBand interconnectivity

SMP Servers – two

Each with 16 cores, 72 GB RAM

Storage & Backup:

15 TB usable storage space over the NFS mount.
NAS servers being used to mount storage.
50X1.6 TB Tape Library capacity for Backup.

Software

HPC: OFED, Mvapich, mpich, Intel Compilers, Windows HPC pack 2008, Python 3.1

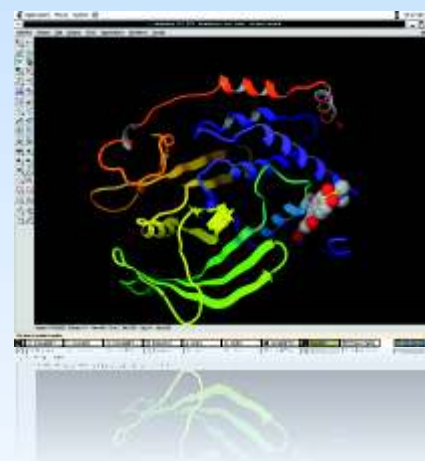
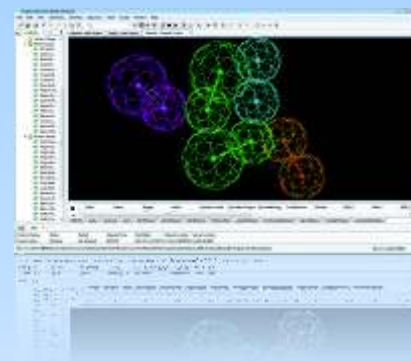
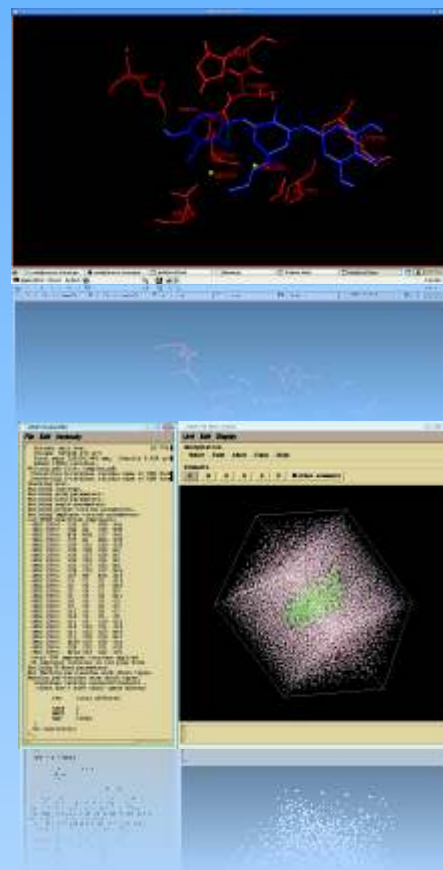
Scheduling & management software: PBS-Pro & e-BioChem

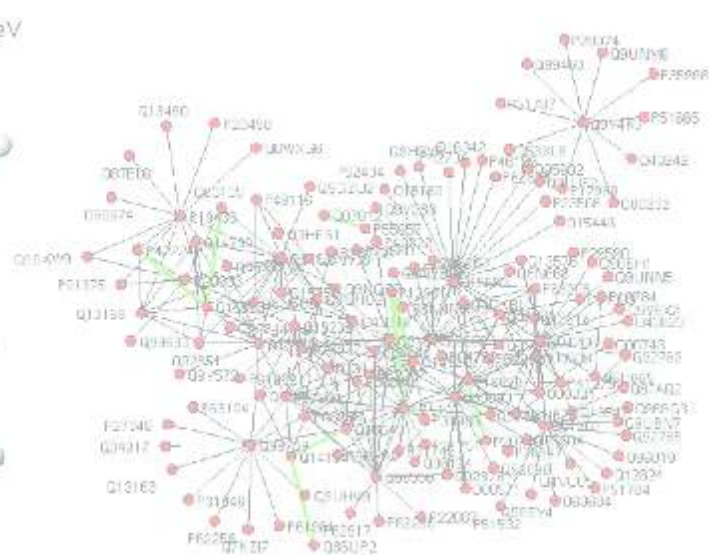
Software for pharmaceutical research:

Amber	-- Molecular dynamics
AutoDock	-- Molecular docking
CPMD	-- Quantum molecular dynamics
Discovery Studio	-- Molecular modeling suite
Gaussian	-- Quantum chemical analysis
GROMACS	-- Molecular dynamics
Maestro	-- Chemical simulation software
MATLAB	-- Artificial Intelligence and simulations
MOE	-- Bioinformatics and chemoinformatics
NAMD	-- Molecular dynamics
OpenEye	-- Molecular modeling and chemoinformatics
Pipeline pilot	-- Workflow analysis
SPSS	-- Statistical analysis
StarDrop	-- Drug metabolism analysis
Sybyl	-- Molecular modeling suite
VASP	-- Quantum molecular dynamics
... and many more.	

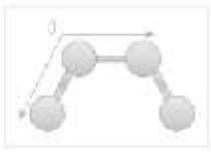
Network Connectivity

The objective is to provide the necessary infrastructure to obtain rapid access to information and computing resources locally and globally. This is accomplished by establishing a high-speed network within the Institute to provide national and international connectivity.

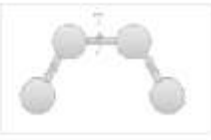




$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$$



Torsion Energy $E_{\text{torsion}} = E_{\text{torsion}}^0 [1 + 0.5 (1 + \cos(\theta))]$

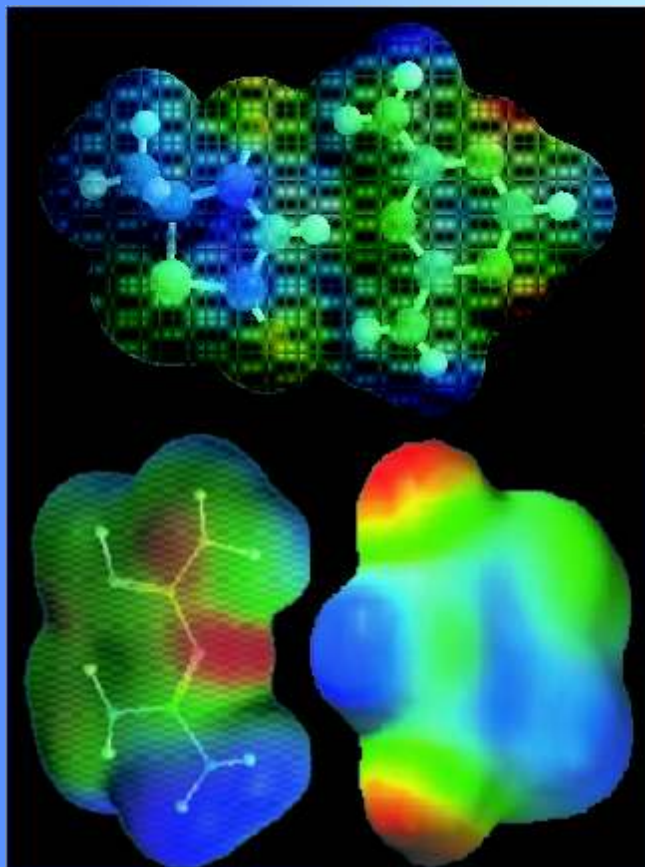


Bending Energy $E_{\text{bending}} = E_{\text{bending}}^0 [1 + 0.5 (1 + \cos(\theta))]$

Molecular Dynamics and Monte Carlo Free Energy Calculations

$\Delta G^\circ = -RT \ln K_{\text{eq}}$

$\Delta G^\circ = -RT \ln(P_2/P_1) = -RT \ln(f_2/f_1)$ where



Energy (E) = $E_{\text{Stretch}} + E_{\text{Bending}} + E_{\text{Torsion}} + E_{\text{Non-bonded Interactions}}$

Stretching Energy: $E_{\text{stretch}} = \frac{1}{2} k_s (r - r_0)^2$



Bending Energy: $E_{\text{bending}} = \frac{1}{2} k_b (\theta - \theta_0)^2$



Activities

- QSAR Analysis for Ligand Based Drug Design
- Pharmacophore Mapping Analysis for Ligand and Receptor Based Drug Design
- Target Discovery for Structure Based Drug Design
- Molecular Docking for Structure Based Drug Design
- *De Novo* Design for Structure Based Drug Design
- Comparative Genomics Studies
- Computational ADME/T Predictions of Drug Like Molecules
- Computational Analysis of Clinical Data
- Computational Modeling of Drug Stability
- Computational Modeling of *in vitro* and *in vivo* Processes
- Computer Aided Analysis of Drug-Drug Interactions
- Computer Aided Analysis of Drug-Excipient Interactions
- Computer Aided Analysis of Organic Reaction Studies for Drug Synthesis
- Computer Aided Drug Delivery Analysis
- Computer Simulations on Macromolecules and their Complexes with Drugs
- Data Mining and Pattern Recognition Studies
- Development of Pharmaceutically Important Databases
- High Throughput Virtual Screening of Different Small Molecule Databases
- Pharmacokinetics-Pharmacodynamics Prediction
- Protein Function Prediction
- Quantum Chemical Analysis of Drugs and Metabolites
- Sequence Analysis and Homology Modeling
- Statistical Analysis of Drug Distribution Systems
- Structural Bioinformatics Analysis of Different Drug Targets
- Systems Biology Analysis of Biomolecules, Tissues, Organs, Organisms, etc.

National Institute of Pharmaceutical Education and Research, S.A.S. Nagar (NIPER-S)

National Institute of Pharmaceutical Education and Research, S.A.S. Nagar (NIPER-S) is the first national level institute in pharmaceutical sciences with proclaimed objective of becoming a centre of excellence of advanced studies and research in pharmaceutical sciences. The Government of India declared NIPER-S as an 'Institute of National Importance' by an act of Parliament in 1998. It is an autonomous body under the Department of Pharmaceuticals (DoP), Ministry of Chemicals and Fertilizers, Government of India. The Institute is conceived to provide leadership in pharmaceutical sciences and related areas not only within the country, but also to the countries in South East Asia, South Asia and Africa. NIPER-S is a member of Association of Indian Universities and Association of Commonwealth Universities.

Objectives

The main objectives of the Institute are:

- To nurture and promote quality and excellence in pharmaceutical education and research
- To tone up the level of pharmaceutical education and research by training the future teachers, research scientists and managers for the industry and profession
- To create National Centres to cater to the needs of pharmaceutical industries and other research and teaching institutes
- To collaborate with Indian industries to meet the global challenges in pharma research
- To develop curriculum and media
- To conduct continuing education programs for teachers, pharmaceutical technologists, community and hospital pharmacists and other professionals in pharmaceutical field
- To create a central facility of pharmaceutical instrumentation and pharmaceutical analysis for use by the researchers within and outside the institute
- To develop an informatics centre to cater to the needs of researchers within and outside the institute
- To develop a centre with state of the art facilities for creation of new knowledge and transmission of existing information in pharmaceutical areas
- To organize national and international symposia, seminars and conferences in selected areas of pharmaceutical education from time to time
- To act as nucleus for interaction between academia and industry by encouraging exchange of scientists and other technical staff between the institute and industry
- To undertake sponsored and funded research as well as consultancy projects
- For further information on other central facilities in the Institute, please visit: www.niper.gov.in



National Institute of Pharmaceutical Education and Research (NIPER-S)

Sector 67, S.A.S. Nagar (Mohali) Punjab - 160 062
Tel.: 91-172-2214682-2214687 Fax: 91-172-2214692
E-mail: pharmagrid@niper.ac.in
Website: www.niper.gov.in

