



Philippine e-Science Grid Initiatives

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Technology Institute



Outline

- Current Researches
- Proposed Program
 - Philippine e-Science Grid
 - Implementation of Projects
 - Potential Beneficiaries

About ASTI

The Advanced Science and Technology Institute conducts scientific research and development in the advanced fields of Information and Communications Technology and Microelectronics.

Agricultural Biotechnology

- **Development of molecular markers**
- **Discovery of important genes and their regulatory elements**
- **Plant transgenesis**
- **Regulation of GM crops as part of science-based risk assessment**
- **Most of the R&D activities are based at the University of the Philippines Los Baños (IPB, BIOTECH, IBS), PCARRD, PCMARD, PhilRice & IRRI**

Agricultural Biotechnology

- K-AgriNet Program
Knowledge Networking Towards Enterprising
Agricultural Communities
(PCARRD-DOST, DA-PhilRice, DAR & DAP)
- FITS
Farmer's Information and Technology Services
Information System Centers
(PCARRD - DOST)

Medical Bioinformatics

- **Population screening**
- **Drug discovery and development**
- **Outbreak detection**
- **Disease characterization**
- **Vaccine development**
- **Analysis of results and data mining & management (PCR primer design, nucleotide sequence alignment, sequence analysis, phylogeny, protein structure prediction, epitope prediction, etc.)**
- **Most of the R&D activities are based at the University of the Philippines (Manila & Diliman), St. Luke's Medical Center, University of Santo Tomas, RITM – DOH & UNILAB**

Medical Bioinformatics

<http://www.bioinfo.e-health.ph>

- A one-stop-easily navigable health research portal
- An information resources builder in the form of specialty databases, electronic journals, directories, among others
- A venue for research collaboration and information dissemination

Medical Bioinformatics

<http://www.e-health.ph>

- **Health and related news and advisories**
- **Searchable local researcher and research databases**
- **Message board**
- **Relevant health and health research links**
- **SMS messaging (Mobile phone to email application)**
- **Online polls/survey**
- **Content management system**

Telehealth Service Program

- Philippine Council for Health Research and Development (PCHRD- DOST)
- Department of Science and Technology (DOST)
- University of the Philippines Manila
- University of the Philippines Diliman
- University of the Philippines – Philippine General Hospital

Environment

- Improved weather forecasting
- Climate change research
- Pollution monitoring
- Done by PAGASA, Manila Observatory
- PAGASA Interactive Climate and Weather Information Network (PAGASA, ASTI)
- Earthquake and tsunami research (PHIVOLCS)

DNA Sequence Analysis



Extraction



Amplification



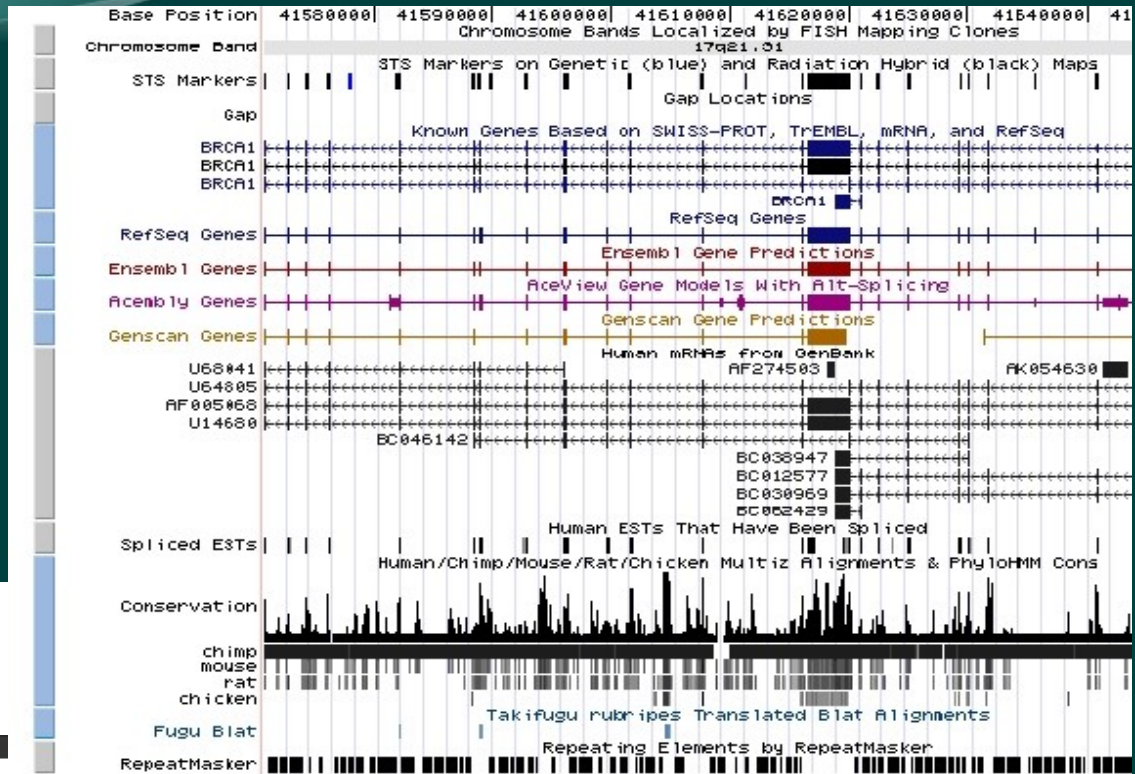
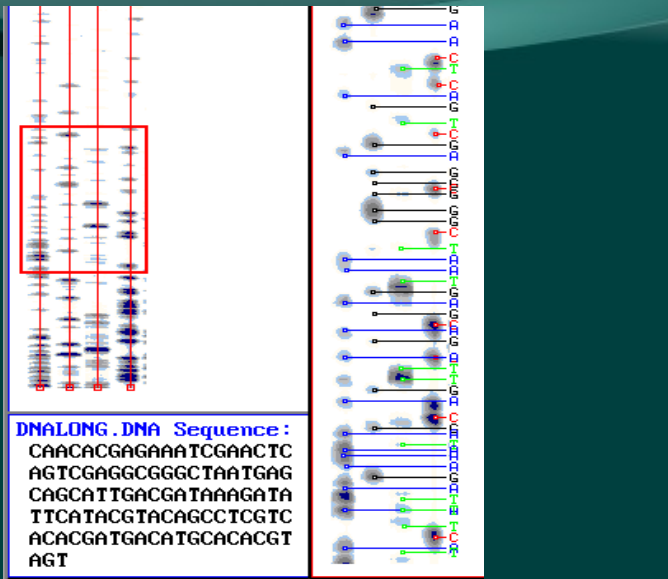
Sequencing



Comparison



DNA Sequence Analysis



Bio-Mirror

- Home
- Contact
- Nodes
- Databases
- Status
- Search GenBank
- Download Rsync Script
- Browse Files

GenBankERS

Search GenBank

Download: AB000060.gb

LOCUS AB000060 2007 bp dna Linear VRL 05-FEB-1999

DEFINITION Feline panleukopenia virus DNA for nonstructural protein 1, complete cds.

ACCESSION AB000060

VERSION AB000060.1 GI:1769777

KEYWORDS nonstructural protein 1.

SOURCE Feline panleukopenia virus.

ORGANISM Feline panleukopenia virus

Viruses; ssDNA viruses; Parvoviridae; Parvovirinae; Parvovirus.

REFERENCE 1 (bases 1 to 2007)

AUTHORS Horiuchi, M.

TITLE Evolutionary pattern of feline panleukopenia virus differs from that of canine parvovirus

JOURNAL Unpublished

REFERENCE 2 (bases 1 to 2007)

AUTHORS Horiuchi, M.

TITLE Direct Submission

JOURNAL Submitted (22-DEC-1996) Motohiro Horiuchi, Obihiro University of Agriculture and Veterinary Medicine, Veterinary Public Health, Inada cho, Obihiro, Hokkaido 080, Japan (E-mail: horiuchi@obihiro.ac.jp, Tel: 0155-49-5392, Fax: 0155-49-5402)

FEATURES

source Location/Qualifiers

1..2007

/db_xref="taxon:10786"

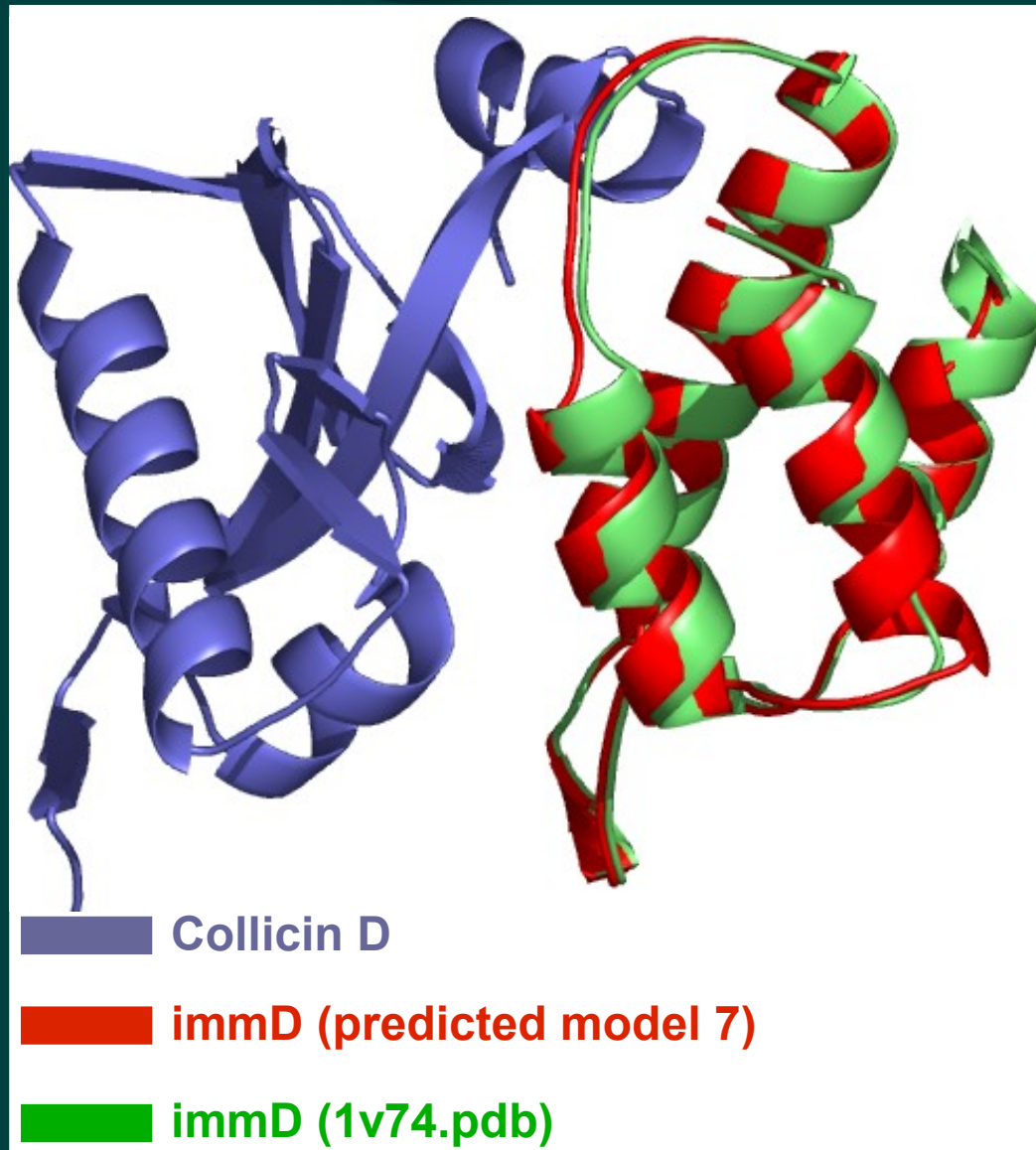
/mol_type="genomic DNA"

/isolate="Som4"

/lab_host="Felis domesticus"

/organism="Feline panleukopenia virus"

Protein Docking



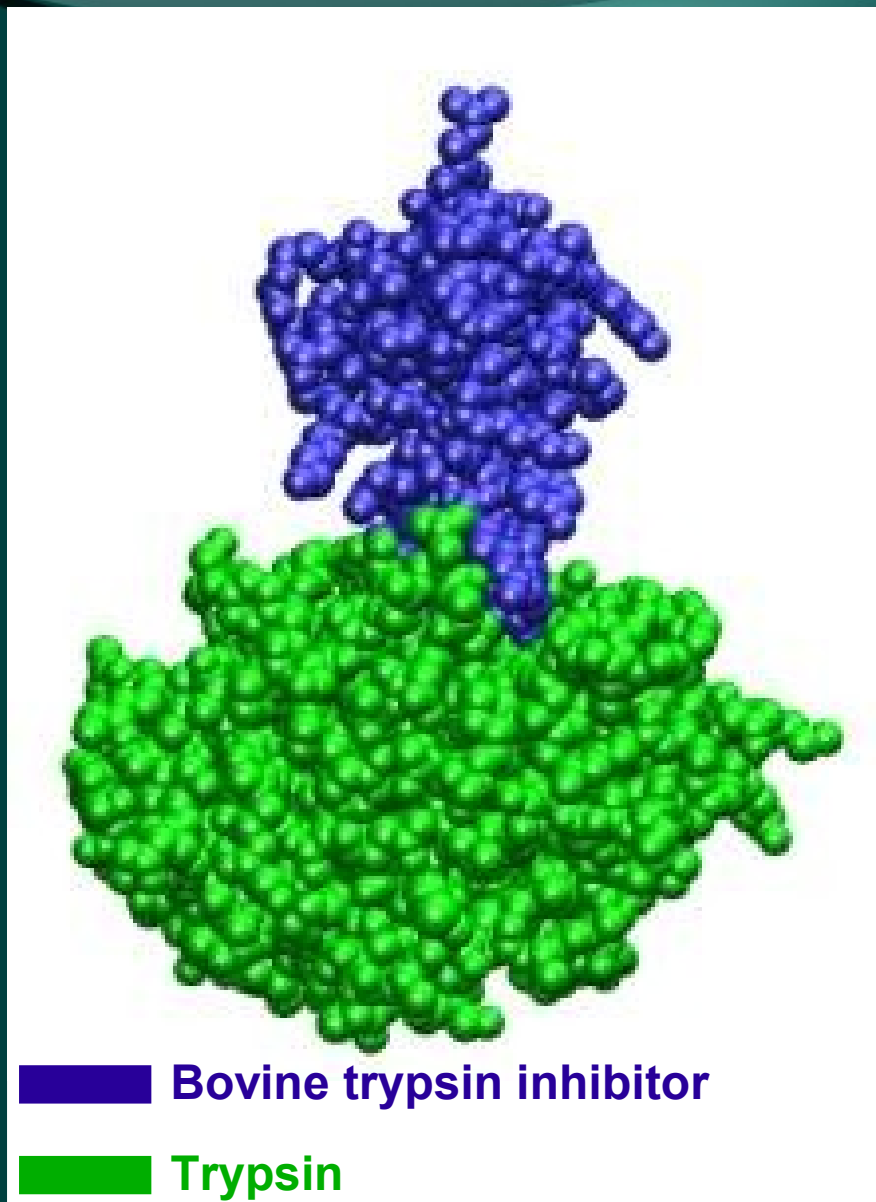
- Collicin immunity protein complex

- Colicin and immunity protein are from *E. coli*.

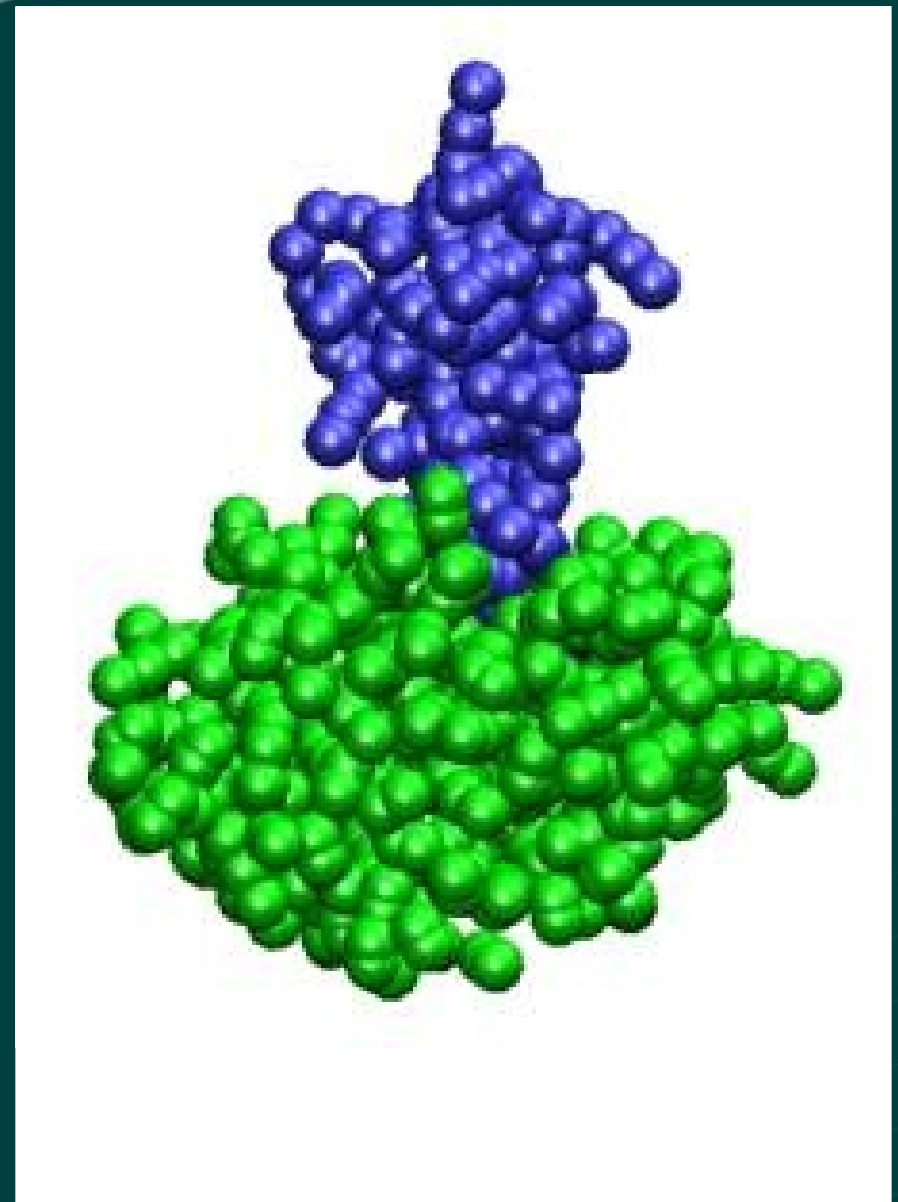
Colicin D is secreted by *E. coli* to kill other bacteria in its medium, and

immD inhibits colicin while it is still in *E. coli* before secretion.

Protein Docking



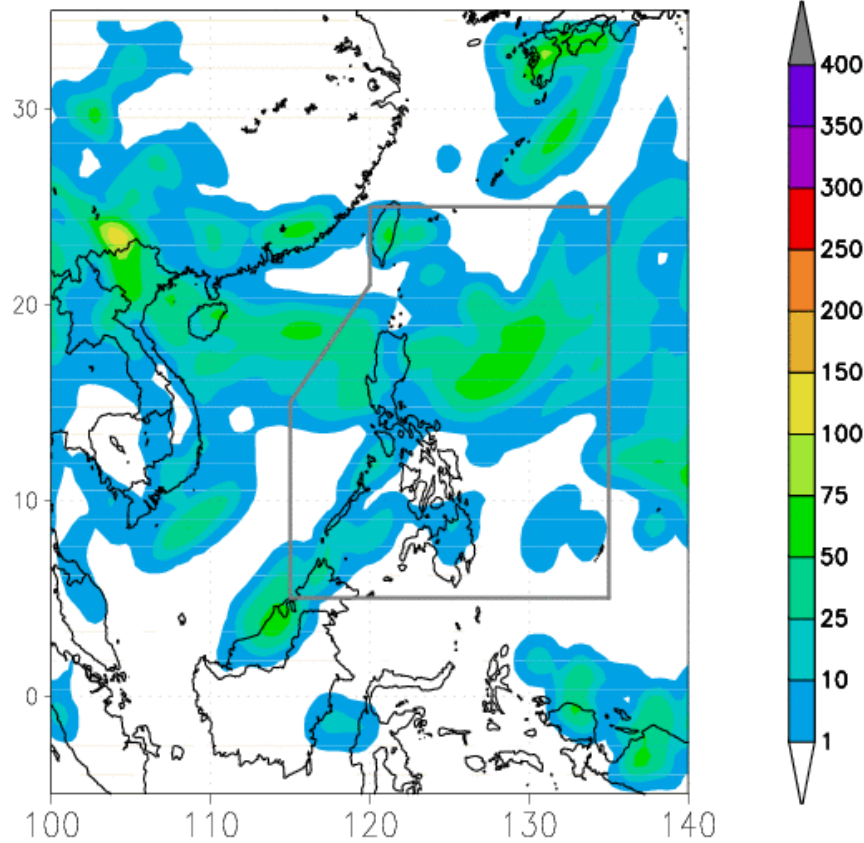
Atomic resolution



Reduced model using pseudo-atoms

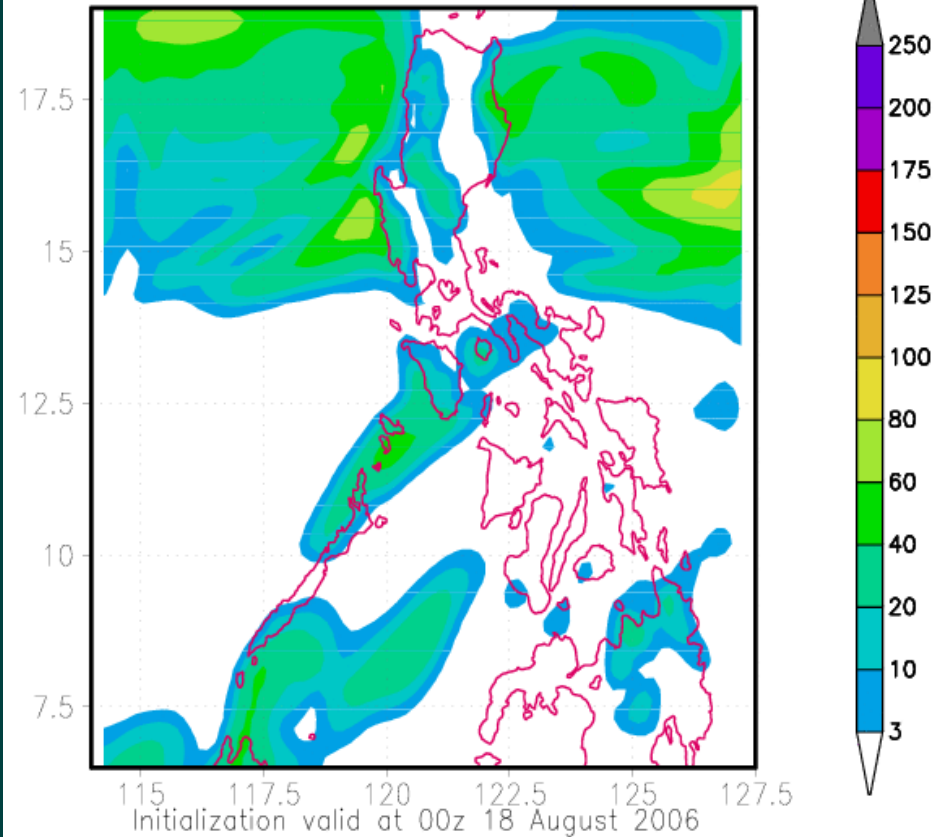
Weather Forecasting: MM5

00–24Hr Acc.Rain (mm) Initialized: 00z 18 August 2006



60 km resolution

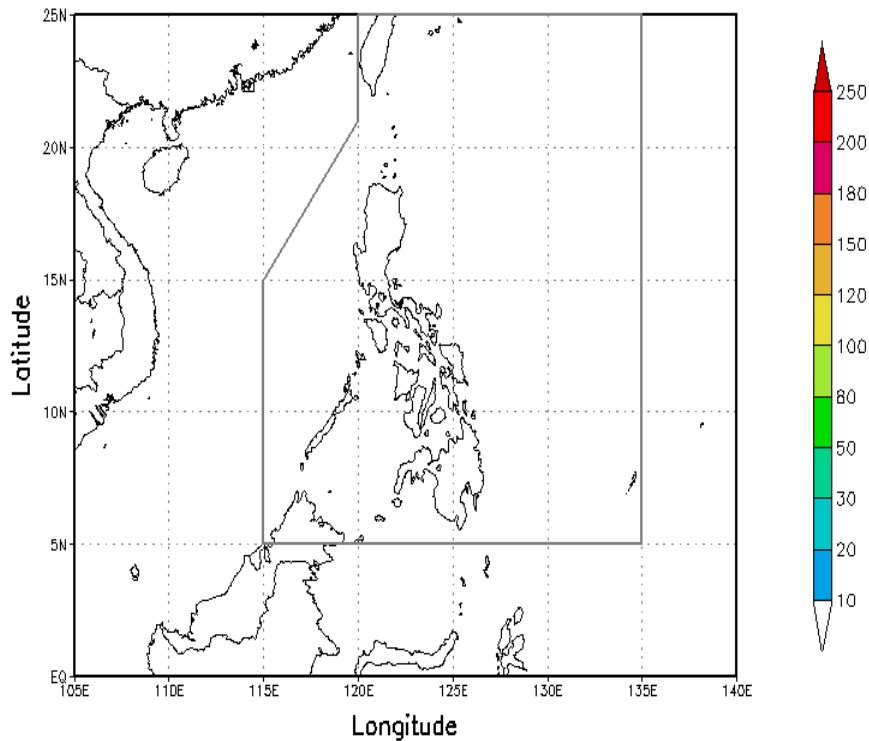
24-hr Accum. Rain (mm)



20 km resolution

Weather Forecasting: HRM

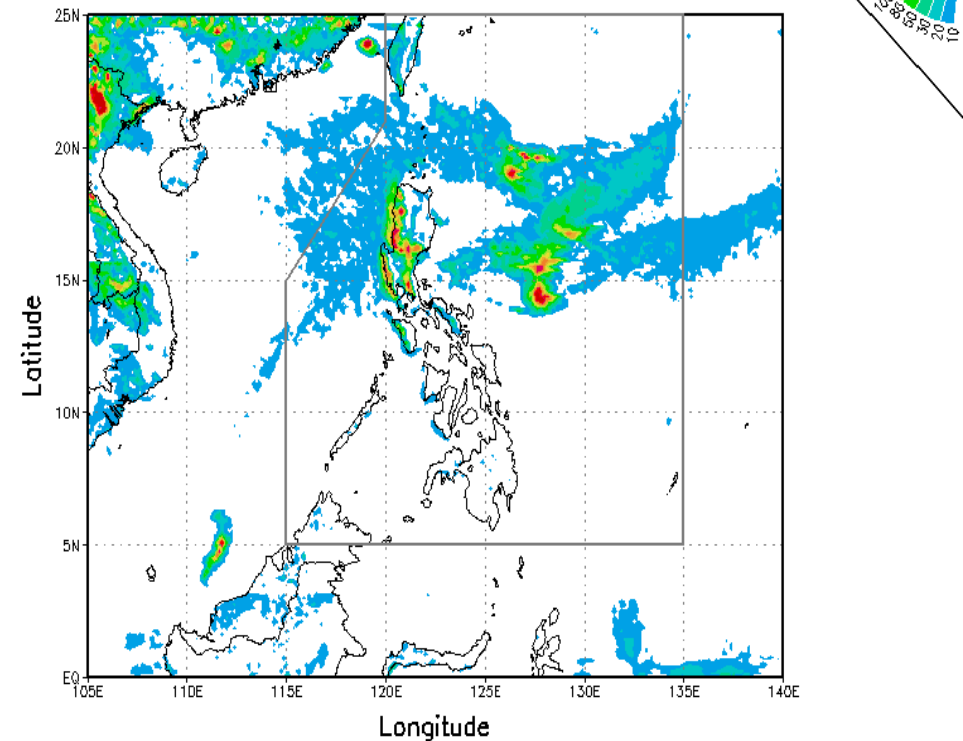
Initial Cumulative Rainfall 0000z 12 SEP 2006
Base Time: 0000z 12 SEP 2006



HIGH RESOLUTION MODEL (HRM)

(Processed by PAGASA/NMG)

24-hr Cumulative Rainfall Prediction for 0000z 19 AUG 2006
Base Time: 0000z 18 AUG 2006



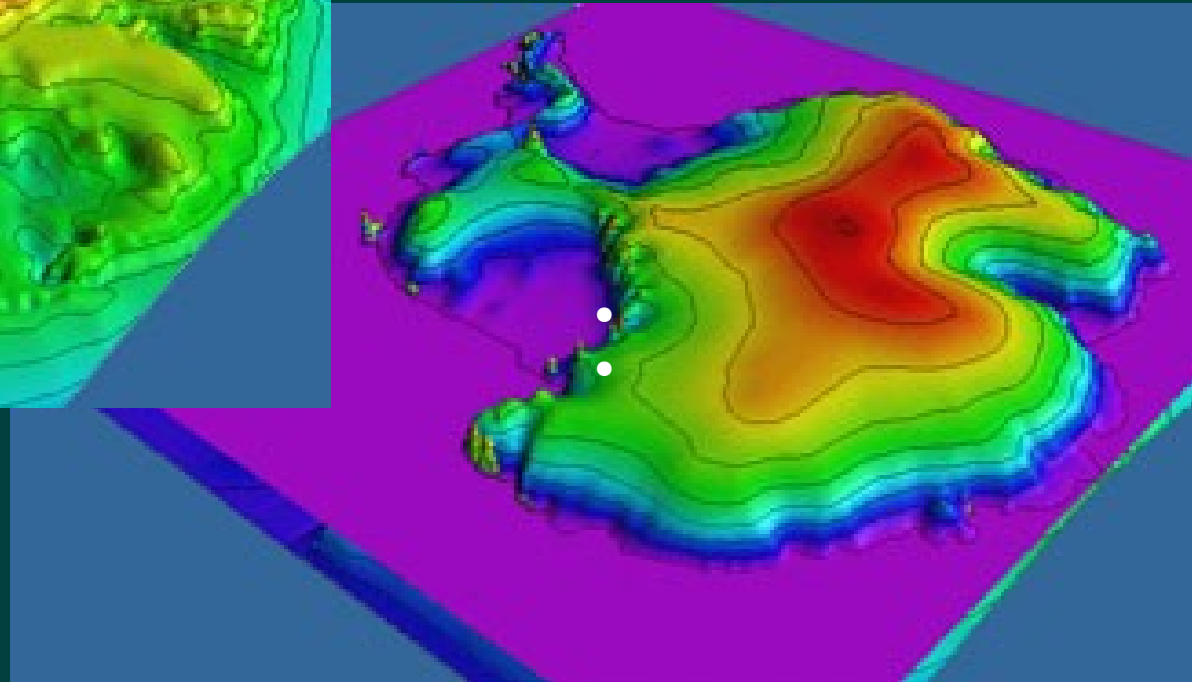
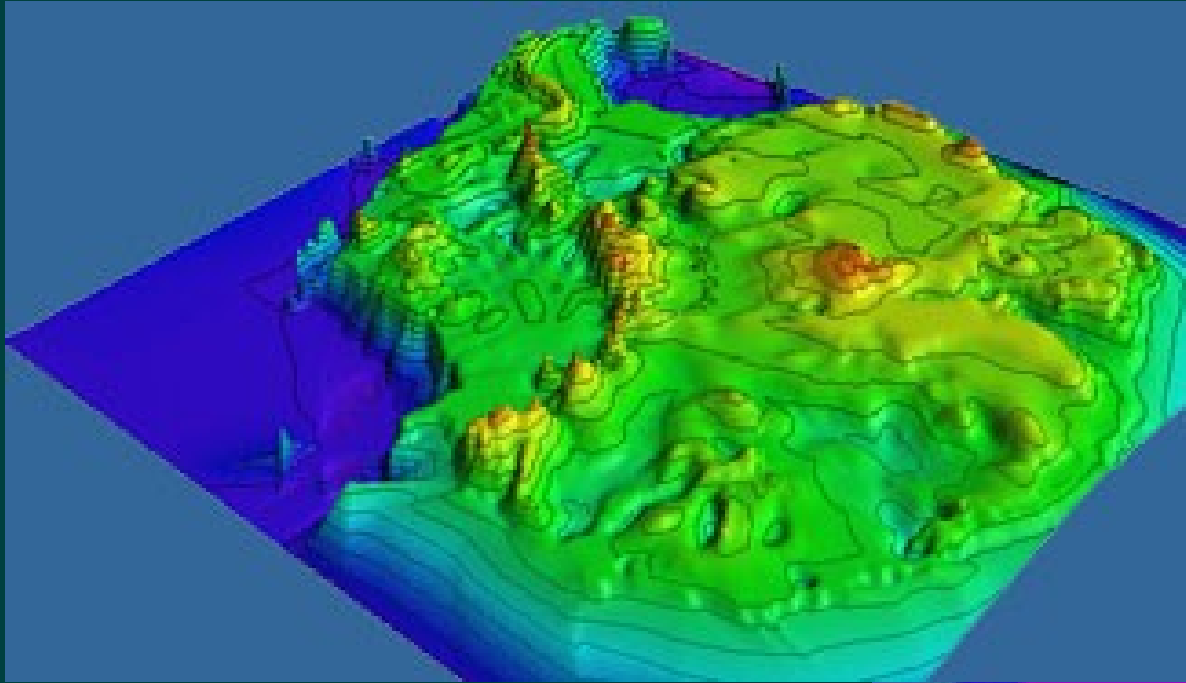
HIGH RESOLUTION MODEL (HRM)

(Processed by PAGASA/NMG)

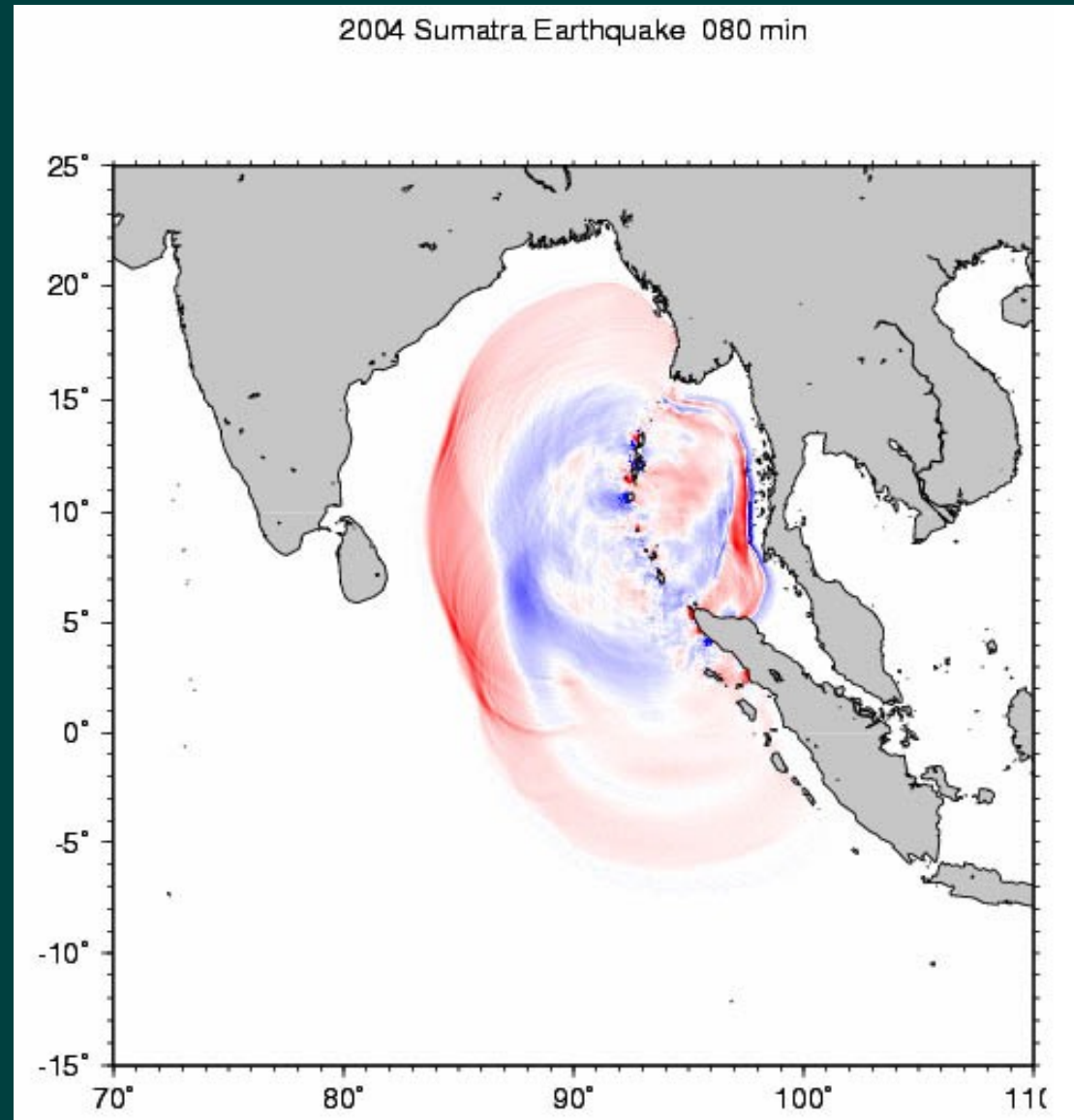
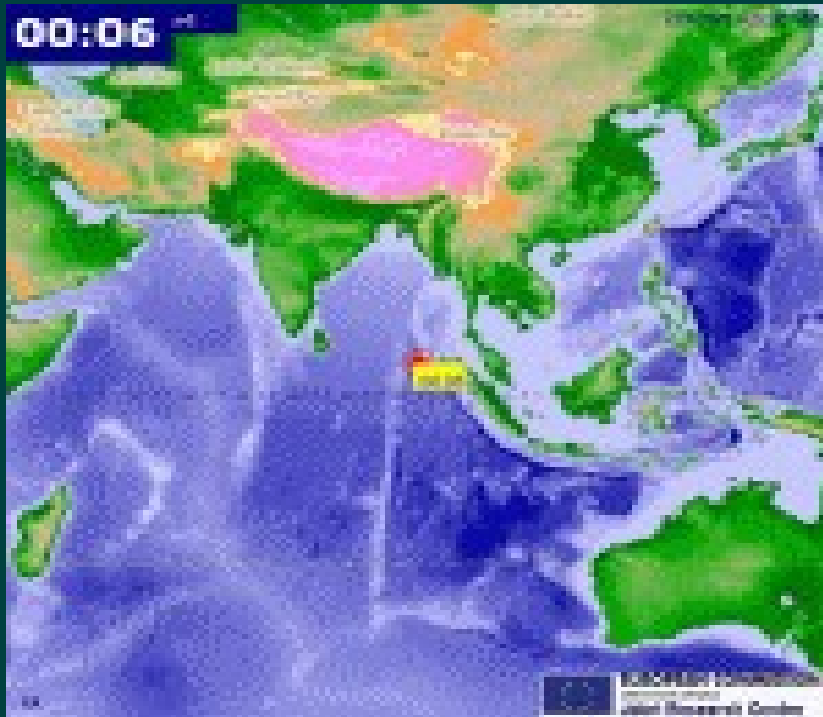
**14 km resolution,
generated in 1hr**

These models (MM5, HRM) still need more improvements to take into account the nuances of Philippine tropical weather.

Climate Modeling



Tsunami Modeling



Challenges of Researchers

- Storage of large data sets as well backup facilities for them
- Operational use reliability
- Organize collaboration between researchers who are dispersed in different institutions
- Dispersed and unstandardized data formats make collaboration difficult
- Scientific visualization

Proposed Project

- Philippine e-Science Grid Program
 - Umbrella program for national grid projects
 - HPC-RC Project
 - Bioinformatics Project
 - Modest goals for year 1
 - Build infrastructure
 - Promote and train researchers in the use of the Grid and HPC resources
 - Lay the ground work for participation in other international grid organizations

Implementation

Philippine e-Science Grid Program

HPC-RC Project

**Bioinformatics
and Computational
Biology Projects**

**Visualization and
Collaborative
Technologies
Projects**

**Environment
and Disaster
Mitigation
Projects**

**Scientific and
Engineering
Computation
Projects**

**Geoinformatics
Projects**



HPC Objectives

- To establish and maintain a high performance computing facility that encourages multi-disciplinary research.
- To organize an advisory committee which will help develop a roadmap on high performance computing.
- To build capability in the field by attending trainings, conferences, and workshops on Cluster/Grid/High Performance Computing, infrastructure, applications,

Standardization

- Common middleware that can “speak” the currently-available formats
- Simplification of code programming, one code => many machines
- Presentation and usage of scientific material, results and tools over the Access Grid
- Federated authentication
 - Institutions can “vouch” for the identity of a user

Data Storage

- Replication of important data to other sites
- Accessibility of data to other researchers
- Updates should propagate automatically

What is the Grid?

- Collection of geographically-dispersed and institutionally-independent computers that may or may not trust each other, but allow users to share computing resources such as CPU time, storage medium, data, etc.

The Grid Today

- Information Grid: World Wide Web
- Data Grid: P2P networks
- Computing Grid: EGEE, OSG, APGrid

Foreign Grids

- National Grid Office (Singapore)
- ThaiGrid (Thailand)
- e-Science Grid Testbed (Malaysia)
- APGrid (Asia-Pacific)
- Enabling Grids for E-scienceE (EU)
- Open Science Grid (US)
- National Research Grid Initiative (Japan)
- NorduGrid (Nordic countries)
- National Center for High Performance Computing (Taiwan)

HPC-RC Project

- Connect HPC clusters in different institutions using a broadband network
- Provide a focal point for Grid services
 - Advisory committee
 - Technical support

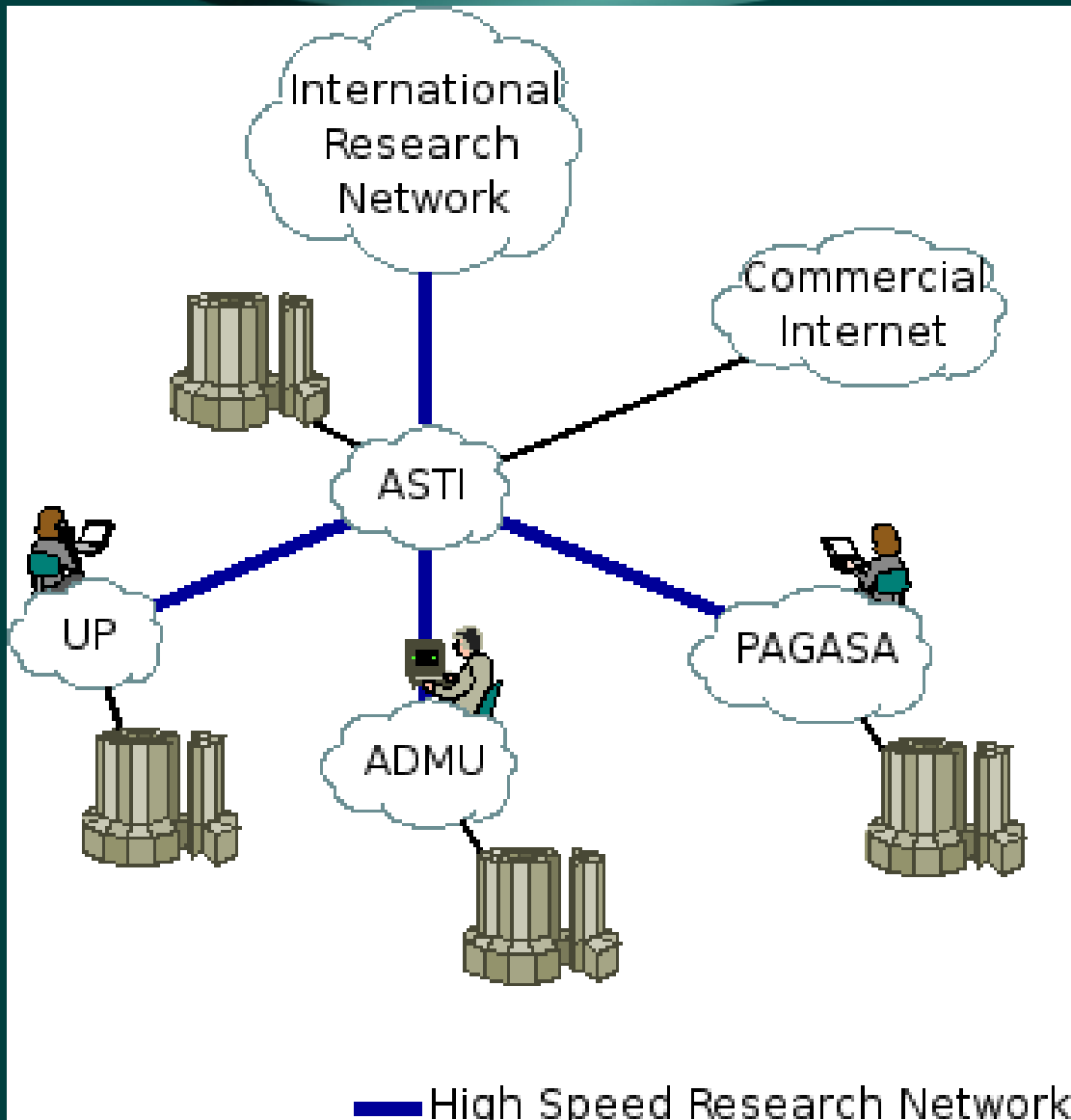
HPC-RC Project

- Advisory board
 - Provide direction, formulate policies
 - Act as liaison in their respective institutions
 - Initial Members:
 - Advanced Science and Technology Institute
 - Ateneo de Manila University
 - Philippine Atmospheric, Geophysical and Astronomical Services Administration
 - University of the Philippines Diliman
 - Limited due to geographic location

HPC-RC Project

- Field-Programmable Gate Arrays
 - reconfigurable architecture
 - supercomputing/hardware

Initial Grid Members



- All conveniently located in Diliman
- High Speed Network will be provided by PREGINET

Bioinformatics Objectives

- To provide rapid access to major biological sequence and structure databases
- To provide a web hosting service for bioinformatics programs to local researchers
- To enhance the expertise of local researchers in bioinformatics

Bioinformatics Project

- Mirror genomic databases from abroad
- Search engine
- Grid workflows
 - Sequence alignment and search
 - Protein docking

Collaborative Tech Project

- Analysis and display systems
- Access Grid integration of technologies for easy collaboration with other researchers

Potential Beneficiaries

- Philippine Interactive Climate and Weather Information Network (PICWIN)
- PHIVOLCS Earthquake and Tsunami Modeling
- National Health Information Network (NHIN)
- Identification of native plants that may have economic value using gene sequencing

Philippine e-Science Grid

Thank you.

<http://philgrid.asti.dost.gov.ph>

References

- The Gray Lab CAPRI Gallery,
<http://graylab.jhu.edu/~mdaily/capri/gallery/gallery.html>
- Protein-protein docking using a reduced model
and accounting for side chain flexibility,
<http://www.iu-bremen.de/schools/ses/mzacharias/08475/>