### Biosciences WG

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### Questions

- What projects the PRAGMA biosciences group are currently working on and what are they interested in pursuing?
  - Is there anything that can be sustained in biosciences with the members and what is the common issue for them?
- Should Biosciences refocus its scientific expedition or integrate projects into existing expeditions?
  - This depends on interest and ability to follow-through.
  - If we create an entirely new expedition, then we need to define the projects/ goals/common issues.
  - If we integrate with existing expeditions, then how can the projects tie-in with the other expeditions?
- What is practically possible, with a focus on funding sources for participants and their ability to participate?
- Can we provide virtual screening as a service for other biologists?
  - Great driver for virtualized network and machines and it leverages on past experience, but is this sustainable and who would use it?
  - Genomics as a driver?

# PRAGMA 27 Summary (1/2)

- Current projects of Biosciences
  - Science Community Laboratory, Thanh Truong
    - Crowdsourced virtual screening (scalability problem)
  - Infectious Disease Bioportal, Nor Arlina Amirah
    - Big data integration, processing, user access
  - SimFlu, Insung Ahn
    - Big data integration, processing, user access
  - ASTI, Jelina Tetangco
    - Works with International Rice Research Institute (IRRI), rice genomics project, 3K genomes
- Should Biosciences refocus or integrate with other expeditions
  - Proteomics
    - Virtual screening/drug discovery
    - Helping to drive resources on PRAGMA-ENT
    - Educational tool, clear link to cyberlearning
  - Genomics
    - Pipeline workflows
    - Infectious disease portals
    - Clear link to biodiversity

# PRAGMA 27 Summary (2/2)

- What is practically possible (funding sources, participation, etc.)
  - Issues
    - Advantage PRAGMA-ENT is breakable
    - Disadvantage PRAGMA-ENT is breakable
    - Need more crosstalk with other groups
    - Genomics is a very large field, we need to be focused
    - Need more genomics domain scientists to develop roadmap
- Bioscience services
  - virtual screening?
  - genomics analysis?

To be continued in Nara...

### SEAIP 2014 – Indonesia Bioscience Activities

- Heru Suhartanto, Arry Yanuar, Universitas Indonesia, Indonesia
   Current Progress on Integrating High Performance Computing Resources,
   Molecular Dynamics Virtual Screening Software, and Database Resources into Cloud Computing Platform to Support Drug Design based on Indonesian Medical Plants
- Kudang B. Seminar, Bogor Agriculture Institute, Indonesia
   An HPC solution for Weed Control Decision Support System Based on Precision Agriculture Approach
- Muhammad Hafizhuddin Hilman, Universitas Indonesia, Indonesia
   Accelerate Massive Data Processing on Virtual Screening Drug Discovery
- Ummi Azizah Rachmawati, Yarsi University, Indonesia
   Yarsi University (Islamic Hospital Foundation) E-health Research
- Yeni Herdiyeni, Bogor Agricultural University, Indonesia IPB Biodiversity Informatics (IPBIOTICS)

# PRAGMA 28 Goals (1/2)

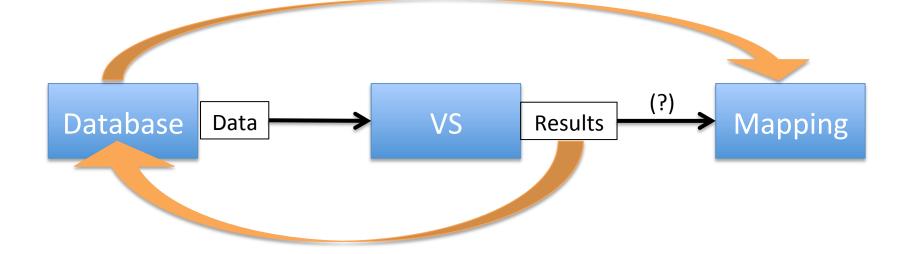
- Establish clearer priorities and goals in two areas
  - Genomics
    - Need to identify area (Tommy Lam, Ly Le)
    - Where to start
      - Deploy standard set of tools to PRAGMA Cloud (?)
      - Create easy to use UI for the tools
    - Involvement of International Rice Research Institute (IRRI), rice genomics project
      - Link to biodiversity efforts

#### Proteomics

- Virtual screening/drug discovery still area of interest with long history
- Natural Products Discovery Portal
  - Can we create a more unified effort
  - Can benefit entire region
  - Identify key partners in this effort

### PRAGMA Natural Products Discovery Platform

- Components
  - 1. Natural products database
  - 2. Virtual screening
  - 3. Biodiversity mapping
- What are the infrastructure requirements for each component?
  - 1. Storage, data format
  - 2. Network, compute nodes
  - 3. Mapping tools, visualization



# PRAGMA 28 Goals (2/2)

- Can these efforts be offered as a service?
  - Academic use
    - Research and teaching tools
  - Industry use
    - Small companies (not large pharma)
  - Policy issues
    - Intellectual property
    - Privacy