



高速運算於生物資訊之應用

HPC for Bioinformatics

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高速運算於生物資訊之應用

HPC for Bioinformatics

PART 1 :

(60 %)

HPC = High Performance Computing

What is HPC? Types of HPC ?

Can I solve my problem with HPC ?

PART 2 :

(30%)

HPC & Bioinformatics Application

PART 3 :

(10%)

Open Source for Bioinformatics



PART 1 :

HPC 101

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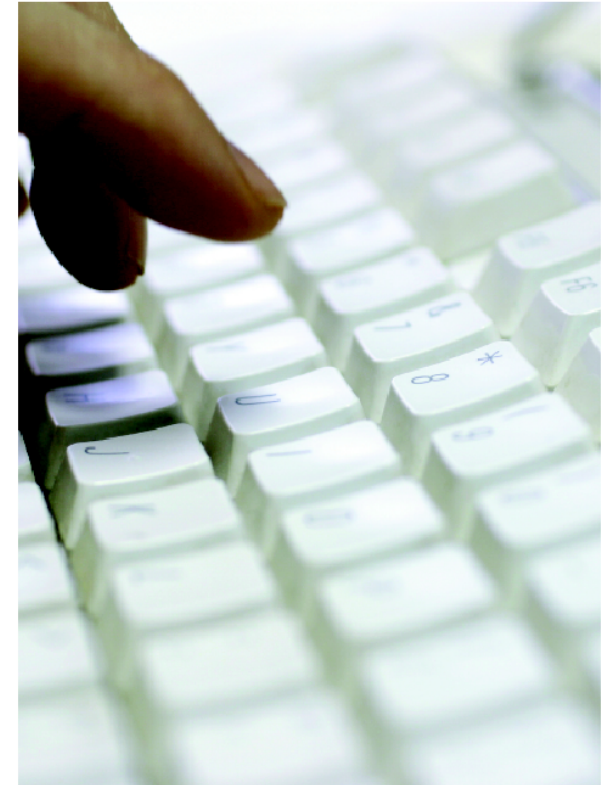
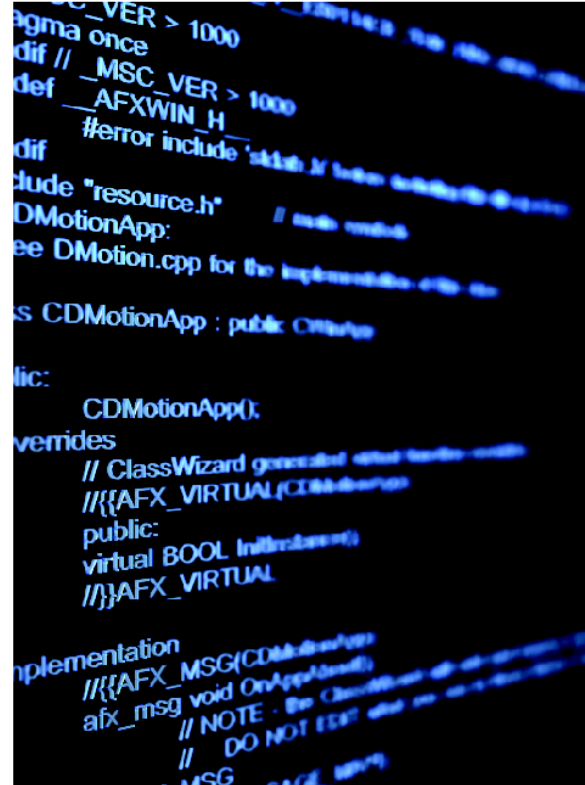
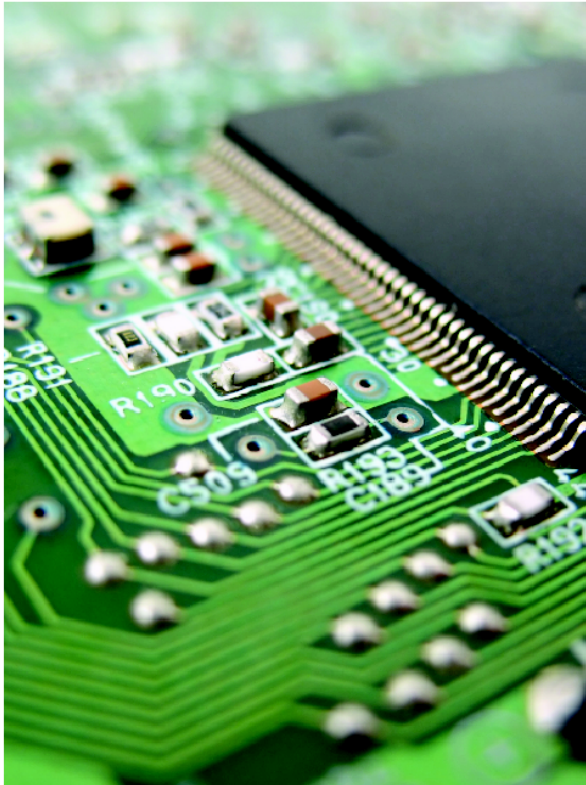


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What is HPC ?

&

Why HPC ?



High performance computing brings together computers, software, and expertise to solve problems too difficult to solve effectively by other means.

Source: <http://insidehpc.com/whatisHPC/WhatIsHPC.pdf>

Simulated crash tests improve auto safety in more scenarios than could be tested in the real world



Too dangerous

Why HPC?

Source: <http://insidehpc.com/whatisHPC/WhatIsHPC.pdf>

www.insideHPC.com/HPCcan

HPC helps find just the right place for tens of thousands of products in stores all over the world



Too time consuming

Why HPC?

Source: <http://insidehpc.com/whatisHPC/WhatIsHPC.pdf>

www.insideHPC.com/HPCcan

HPC helps businesses manage and track billions of packages as they move around the globe



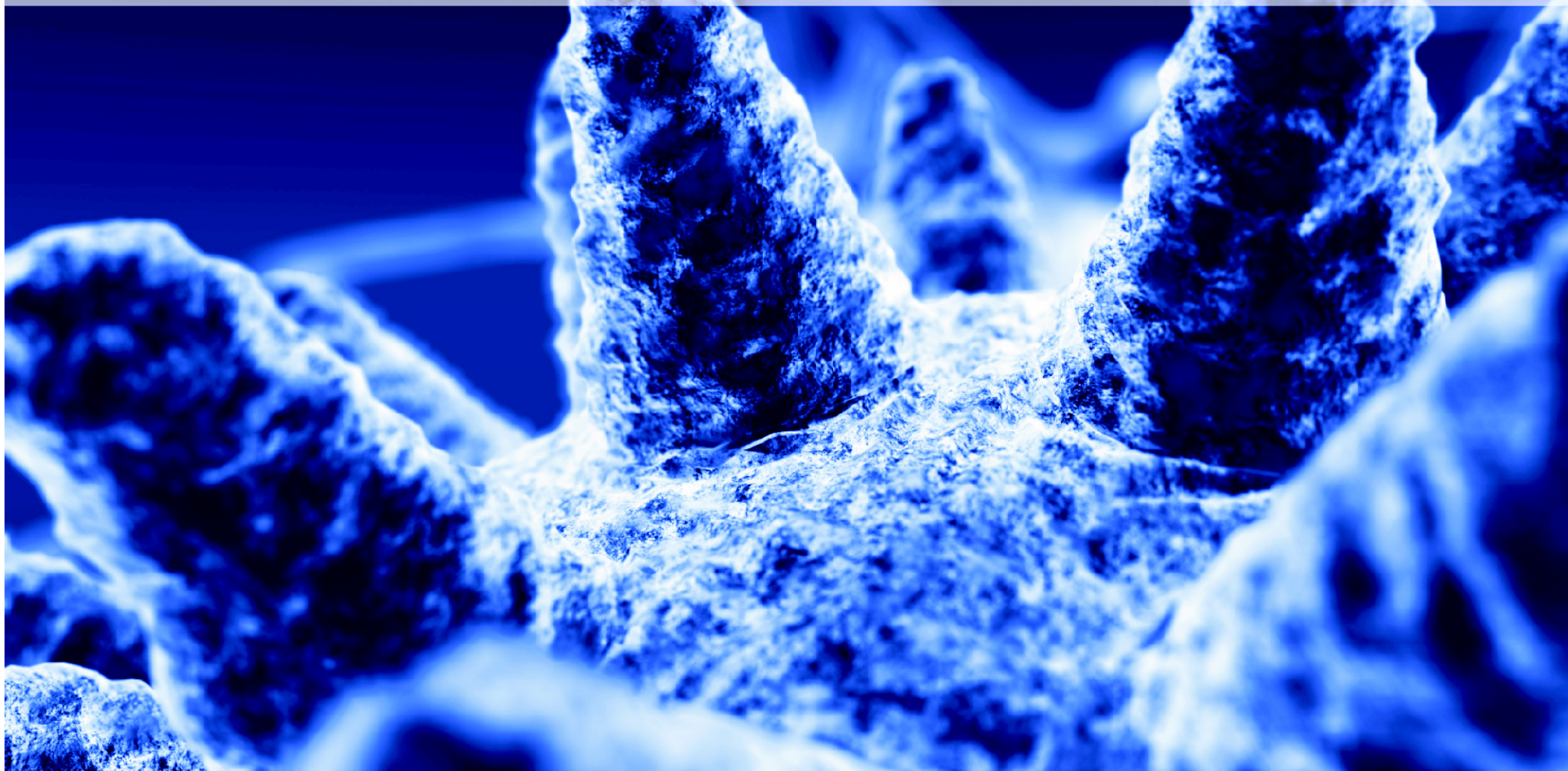
Too complex

Why HPC?

Source: <http://insidehpc.com/whatisHPC/WhatIsHPC.pdf>

www.insideHPC.com/HPCcan

HPC gives doctors and scientists a window into the chemistry of our bodies to help develop new drugs and treatments



Too far beyond other
tools

Why HPC?

Source: <http://insidehpc.com/whatisHPC/WhatIsHPC.pdf>

www.insideHPC.com/HPCcan

Types of HPC ?



Source: http://blog.tice.de/a_icons/icons/512%20Time%20Machine.png

Back to Year 1960s ...

Brief History of Computing (1/5)



1960 PDP-1

*·
·
·*

1965 PDP-7

*·
·
·*

1969 1st Unix

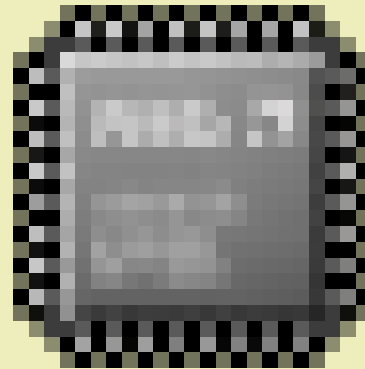
Source: <http://pinedakrch.files.wordpress.com/2007/07/>

***Mainframe
Super
Computer***

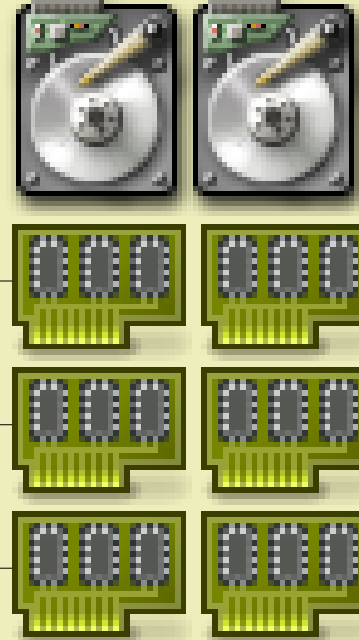
Evolution of Computing Architecture (1/5)



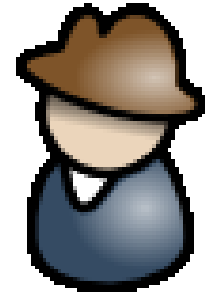
**Multiple
Users**



**Single
CPU**



**Shared
Memory**



**One
Admin.**

**Mainframe
Super
Computer**

**Single
Super Computer**

使用者心裡的『謎之聲』 (1/5)

等執行程式，要排隊排好久喔～

可惡，程式又死掉了，又得重排一次

真希望自己有一台電腦可以跑！！

超級電腦是有錢人才玩得起的玩具～

1977 Apple II

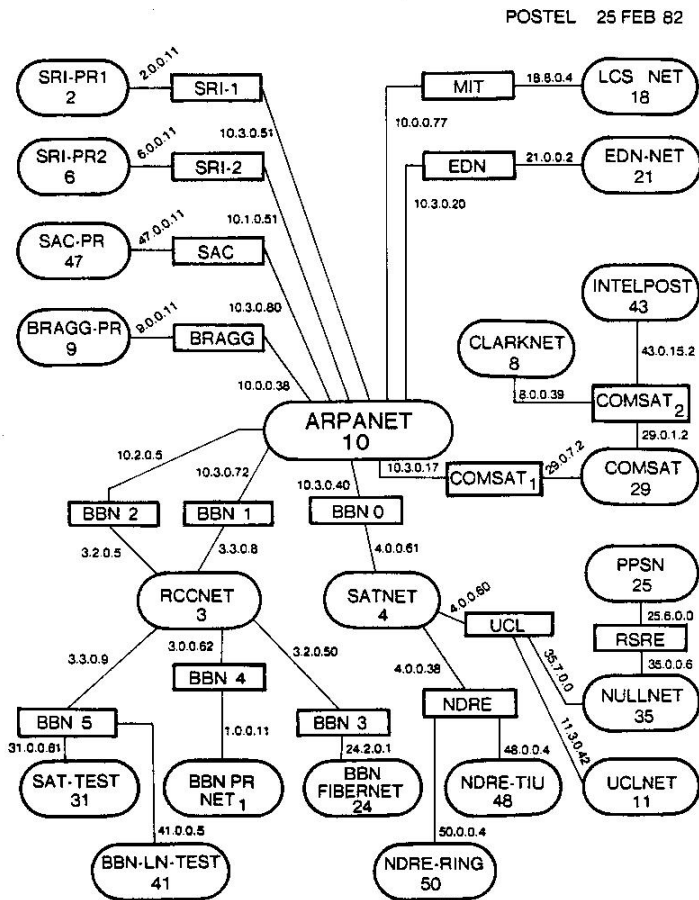


1981 IBM 1st PC 5150

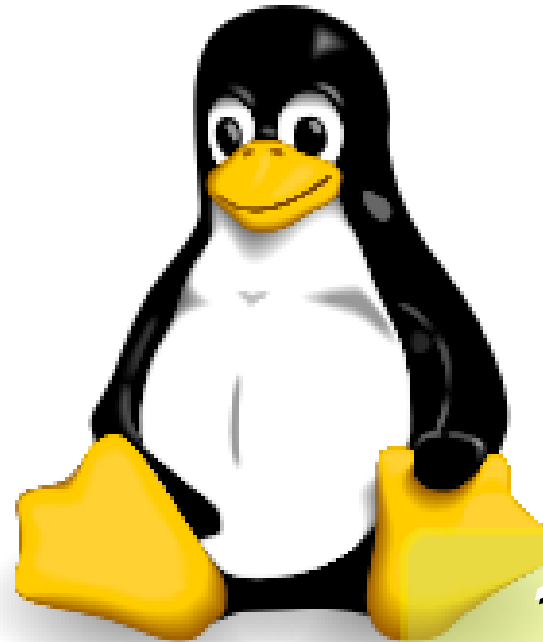


Back to Year 1970s ...

1982 TCPIIP



1983 GNU



1991 Linux

Back to Year 1980s ...

Brief History of Computing (2/5)



Source: <http://www.nchc.org.tw>

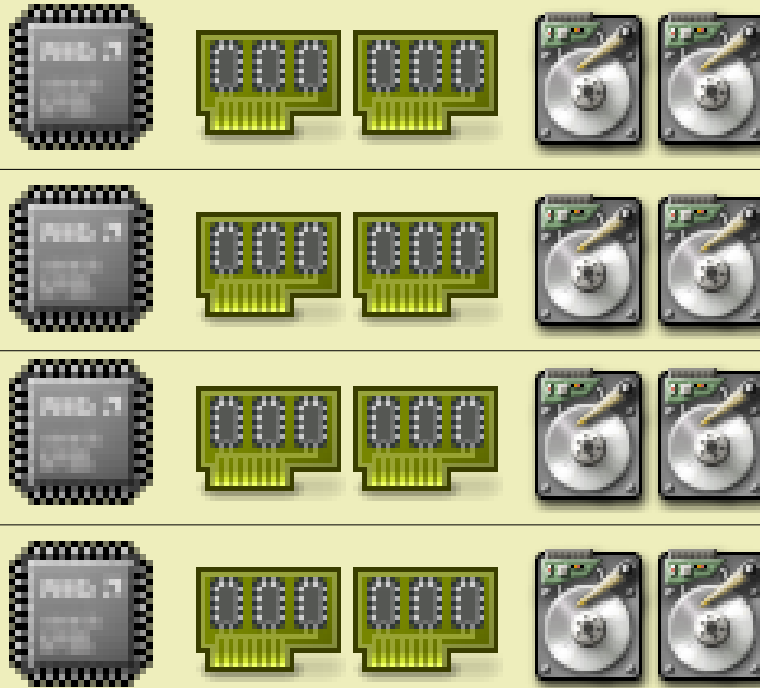
Mainframe
Super
Computer

PC | Linux
Cluster
Parallel

Evolution of Computing Architecture (2/5)

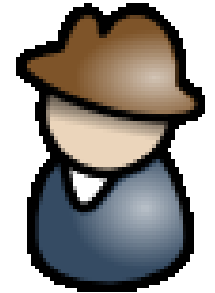


Multiple Users



Separate CPU

Separate Memory



One Admin.

Frame
er
nter

**PC | Linux
Cluster
Parallel**

**Multiple PC
in One Location**

使用者心裡的『謎之聲』 (2/5)

可惡，記憶體不夠大，程式又死掉了

奇怪，我的程式為什麼不能跑？

真希望自己有一組叢集可以跑！！

管理員老大，可以幫我裝 LiBT 嗎？

**1990 World Wide Web
by CERN**

...

...

**1993 Web Browser
Mosaic by NCSA**



1991 CORBA

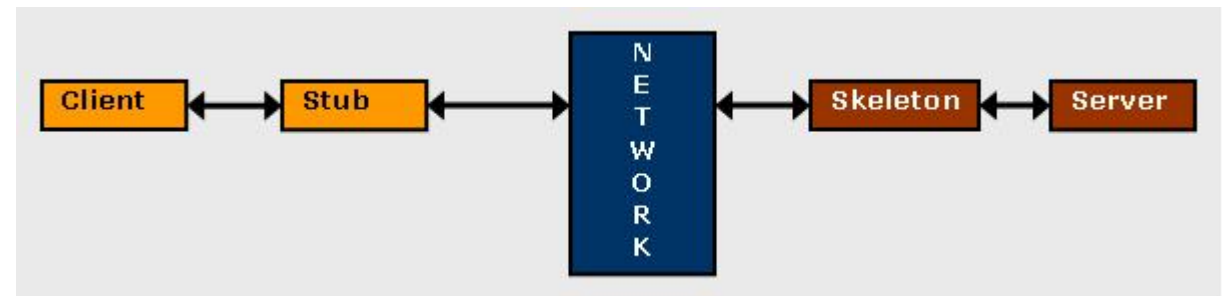
...

Java RMI

Microsoft DCOM

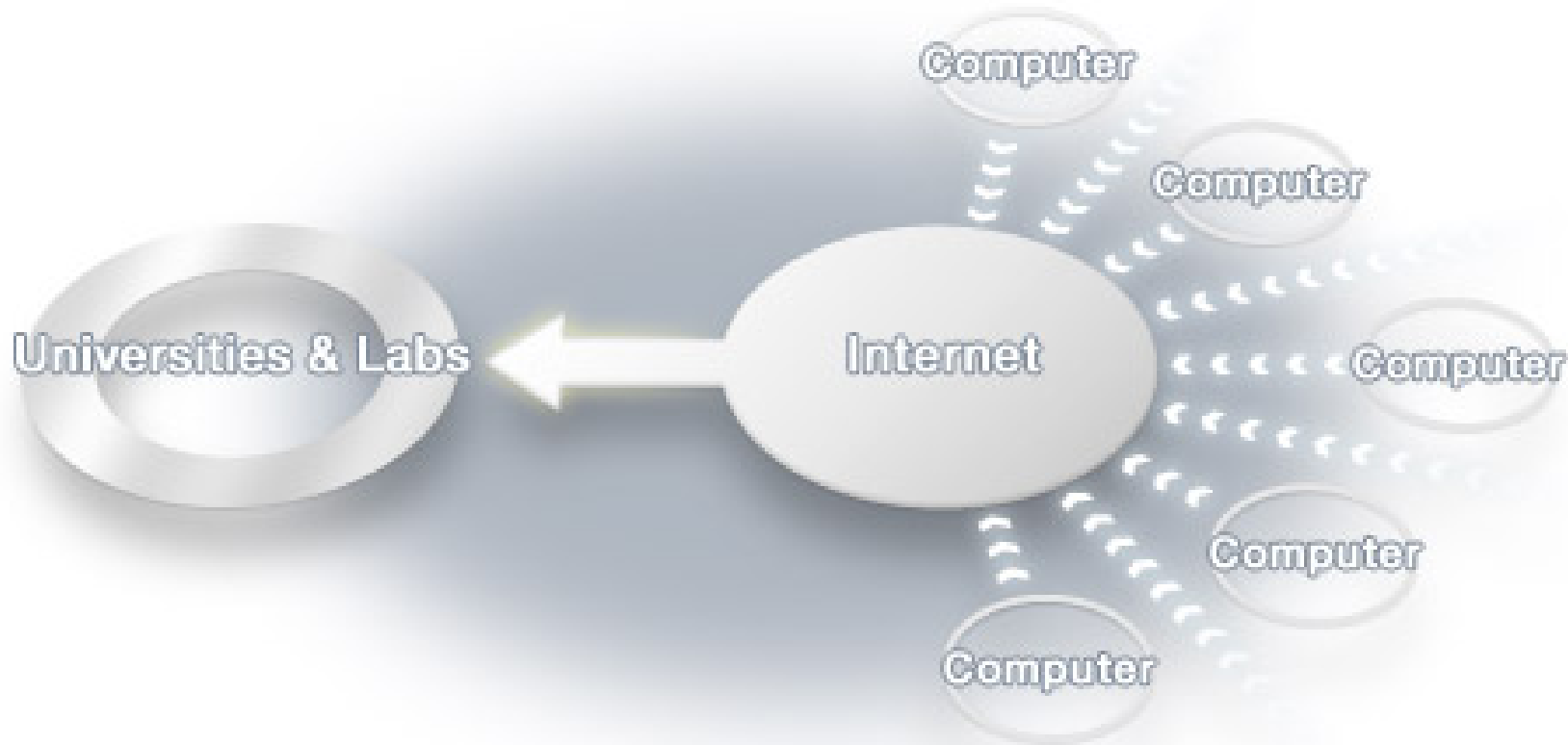
...

Distributed Objects



Back to Year 1990s ...

Brief History of Computing (3/5)



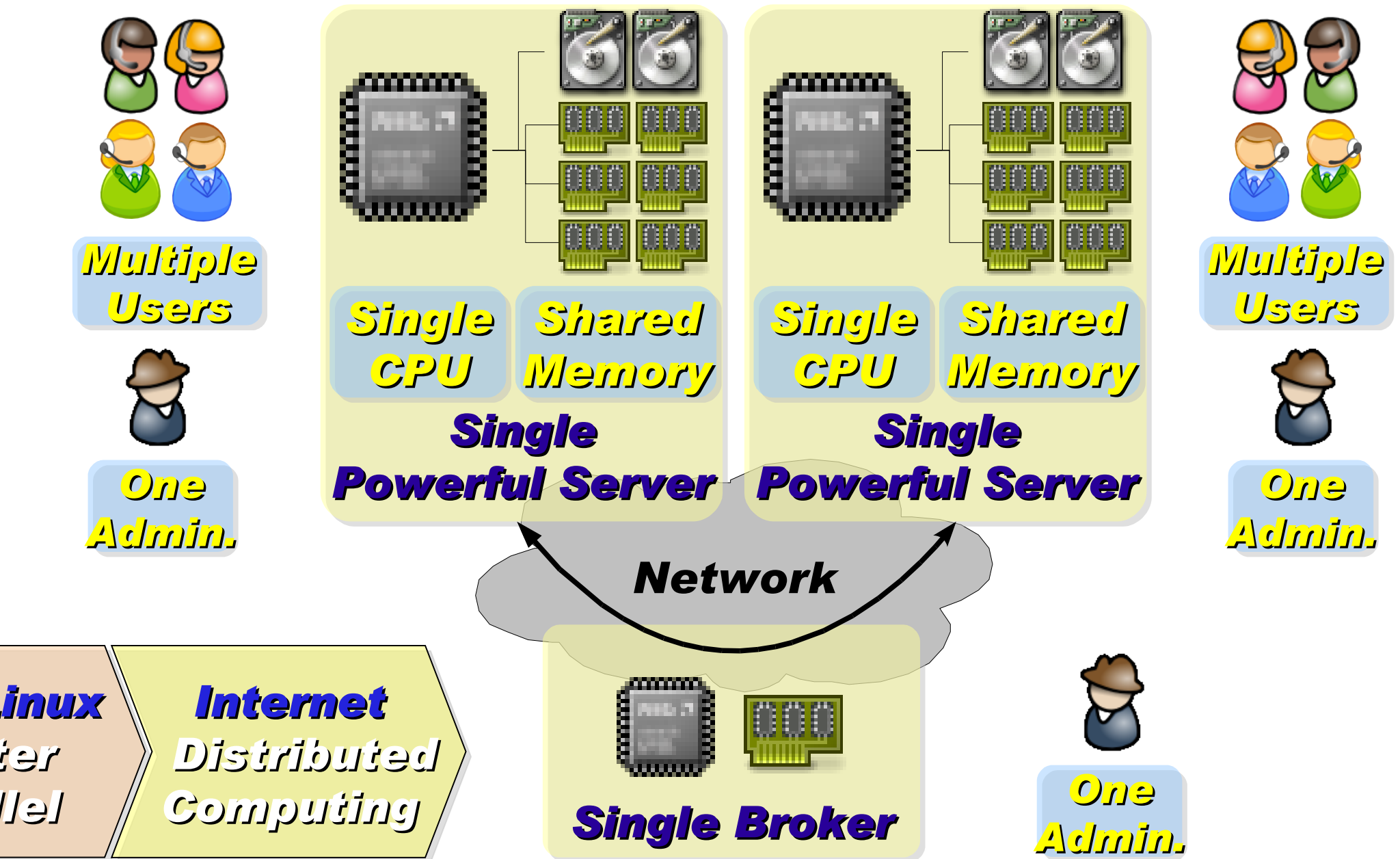
Source: <http://www.scei.co.jp/folding/en/dc.html>

Mainframe
*Super
Computer*

PC | Linux
*Cluster
Parallel*

Internet
*Distributed
Computing*

Evolution of Computing Architecture (3/5)



使用者心裡的『謎之聲』 (3/5)

分散式物件怎麼這麼抽象啊～XD

啊！網路斷線了～不能動了～

大家把閒置電腦都貢獻出來吧！！

給我網路遊戲，其餘免談！

1997 Volunteer Computing
1999 SETI@HOME



2003 Globus Toolkit 2



2002 Berkley BOINC



2004 EGEE gLite



Back to Year 2000s ...

Brief History of Computing (4/5)



Source: <http://gridcafe.web.cern.ch/gridcafe/whatisgrid/whatis.html>

Mainframe
*Super
Computer*

PC | Linux
*Cluster
Parallel*

Internet
*Distributed
Computing*

Virtual Org.
*Grid
Computing*

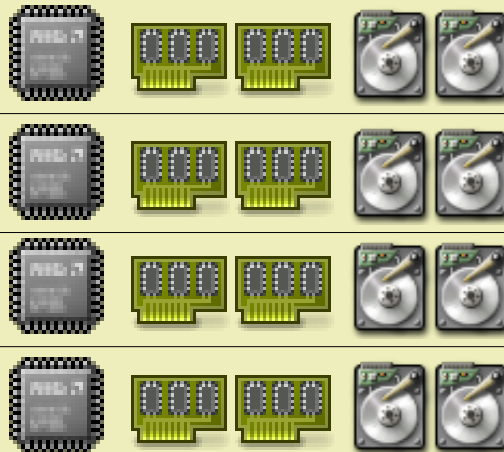
Evolution of Computing Architecture (4/5)



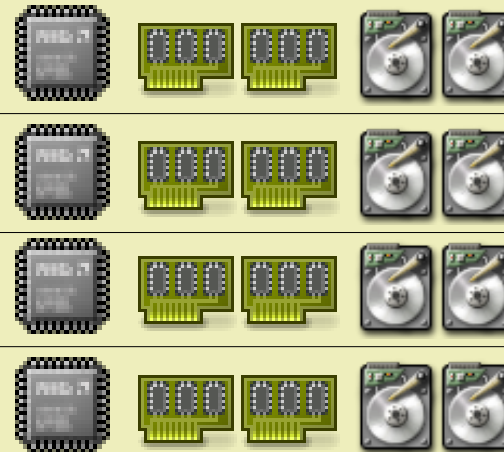
Multiple Users



One Admin.



**Multiple PC
in one location**



**Multiple PC
in other location**



Multiple Users



One Admin.

Grid Middleware

Network

**Internet
distributed
computing**

**Virtual Org.
Grid
Computing**

Virtual Organization

Heterogeneous

CyberInfrastructure

使用者心裡的『謎之聲』 (4/5)

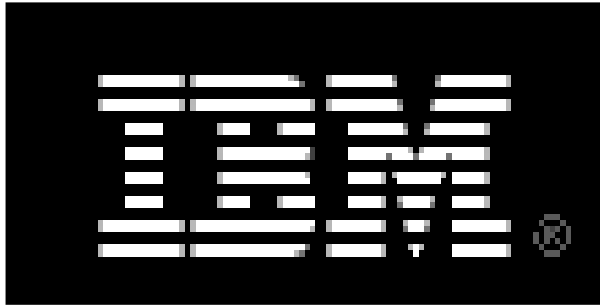
已給我認證了，為什麼要不到資源？

啥？可用資源在美國，慢慢搬檔案吧！

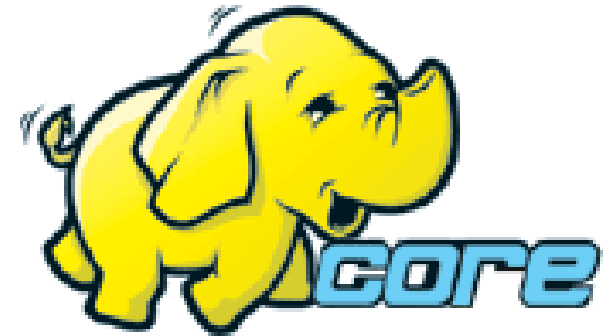
為什麼人家 Google 那麼會算？！

長官，請幫我們去談好資源共享政策吧！

2001 Autonomic Computing
IBM



2006 Apache Hadoop



2005 Utility Computing
Amazon EC2 | S3

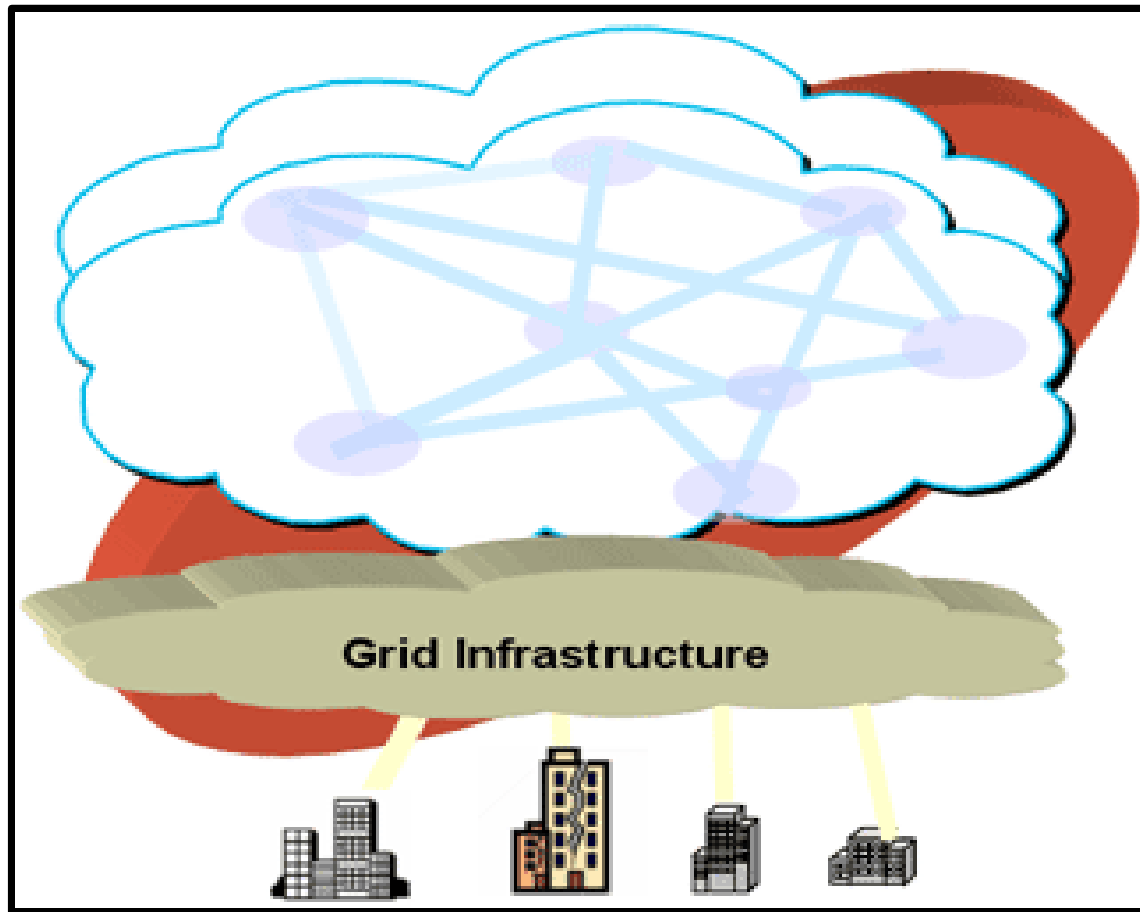


2007 Cloud Computing
Google + IBM



Back to Year 2007 ...

Brief History of Computing (5/5)



Source: <http://mmdays.com/2008/02/14/cloud-computing/>

mainframe
super
computer

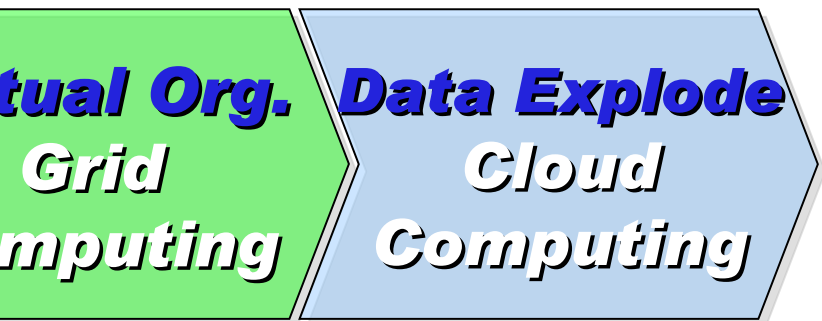
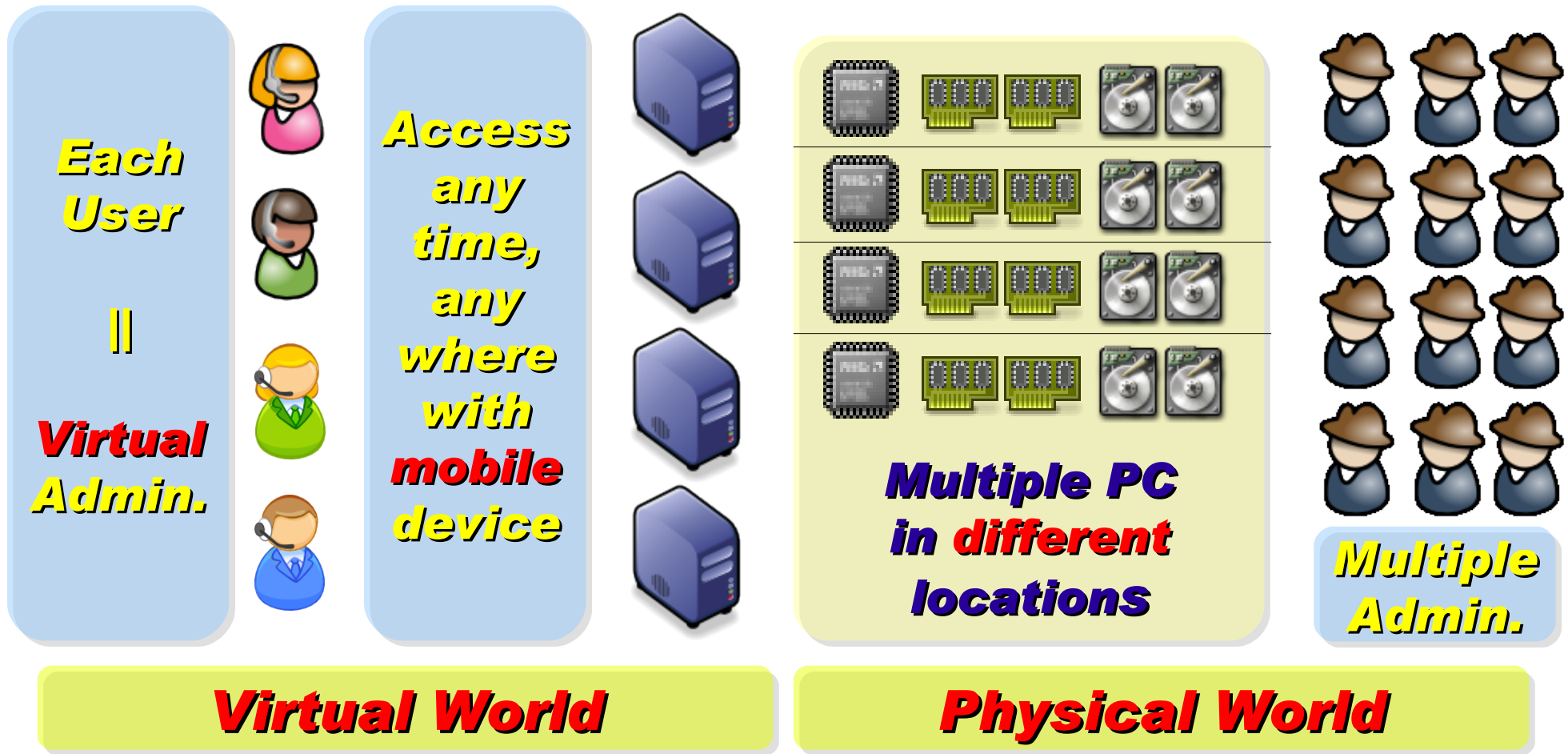
PC | Linux
Cluster
Parallel

Internet
Distributed
Computing

Virtual Org.
Grid
Computing

Data Explode
Cloud
Computing

Evolution of Computing Architecture (5/5)



What is NEXT ?!
Mobile Computing ?!

使用者心裡的『謎之聲』 (5/5)

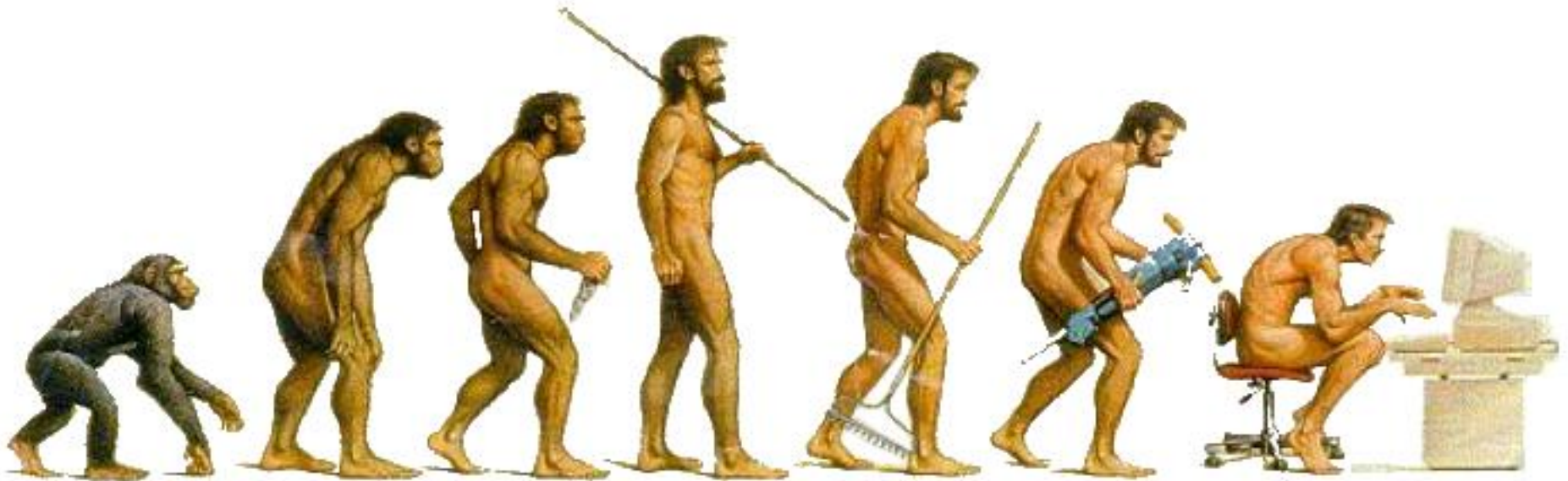
雲端運算合適我用嗎？

按使用時間計費，真的比較省？

Google 到底有沒有偷窺我的信？！

我們自己可以架雲端運算的環境嗎？

Evolution



(OR is it?)

Source: <http://cyberpingui.free.fr/humour/evolution-white.jpg>



Falling to the Ground ...

Source: http://media.photobucket.com/image/falling%20ground/preeto_f10/falling.jpg

**Which Type
of HPC is
the Right ONE
to solve
My Problem ?**



不負責解析

	執行程式 記憶體需求	執行程式 邏輯可分割	輸入資料 數量 / 大小	應用特性 計算特性
超級電腦 Mainframe	非常大 (比 PC 大)	不易分割	單一大檔 GB	即時性高 共享記憶體
叢集運算 Cluster Parallel	小於單一 計算節點 配置量	邏輯相近 可分割	一般數量 MB	即時性一般 共享檔案
分散式運算 Distributed	小於單一 計算節點 配置量	邏輯不同 偕同運作	一般數量 MB	即時性高 訊息傳遞
格網運算 Grid	小於單一 計算節點 配置量	邏輯相近 可分割	一般數量 MB	即時性較低 資料就計算
雲端運算 Cloud	小於單一 計算節點 配置量	邏輯相近 各自獨立	海量檔案 MB	即時性低 計算就資料



PART 2 :

HPC & Bioinformatics Application

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BLAST (*Basic Local Alignment Search Tool*)



- <http://blast.ncbi.nlm.nih.gov/>
- **National Center for Biotechnology Information**
- **BLAST is an algorithm for comparing primary biological sequence information.** (**BLAST** 用來比對生物序列的主要結構)
 - the **amino-acid** sequences of different proteins
 - the **nucleotides** of DNA sequences(例如：不同蛋白質的**氨基酸**序列 **DNA** 序列的**核苷酸**)
- 用途：搜尋其他物種（如：老鼠）未知基因，是否也存在人類基因中
- 優點：使用啟發式搜索來找出相關的序列，比動態規劃快上 **50** 倍。
- 缺點：不能夠保證搜尋到的序列和所要找的序列之間的相關性。
- 技術問題：**巨大的序列資料庫**需要進行比對，怎樣計算才快？
- **Source:** [http://zh.wikipedia.org/w/index.php?title=BLAST_\(生物資訊學\)&variant=zh-tw](http://zh.wikipedia.org/w/index.php?title=BLAST_(生物資訊學)&variant=zh-tw)



PART 2.1 :

Cluster 101 & mpiBLAST

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Powered by DRBL



At First, We have $4 + 1$ PC Cluster

*It'd better be
2ⁿ*



*Manage
Scheduler*

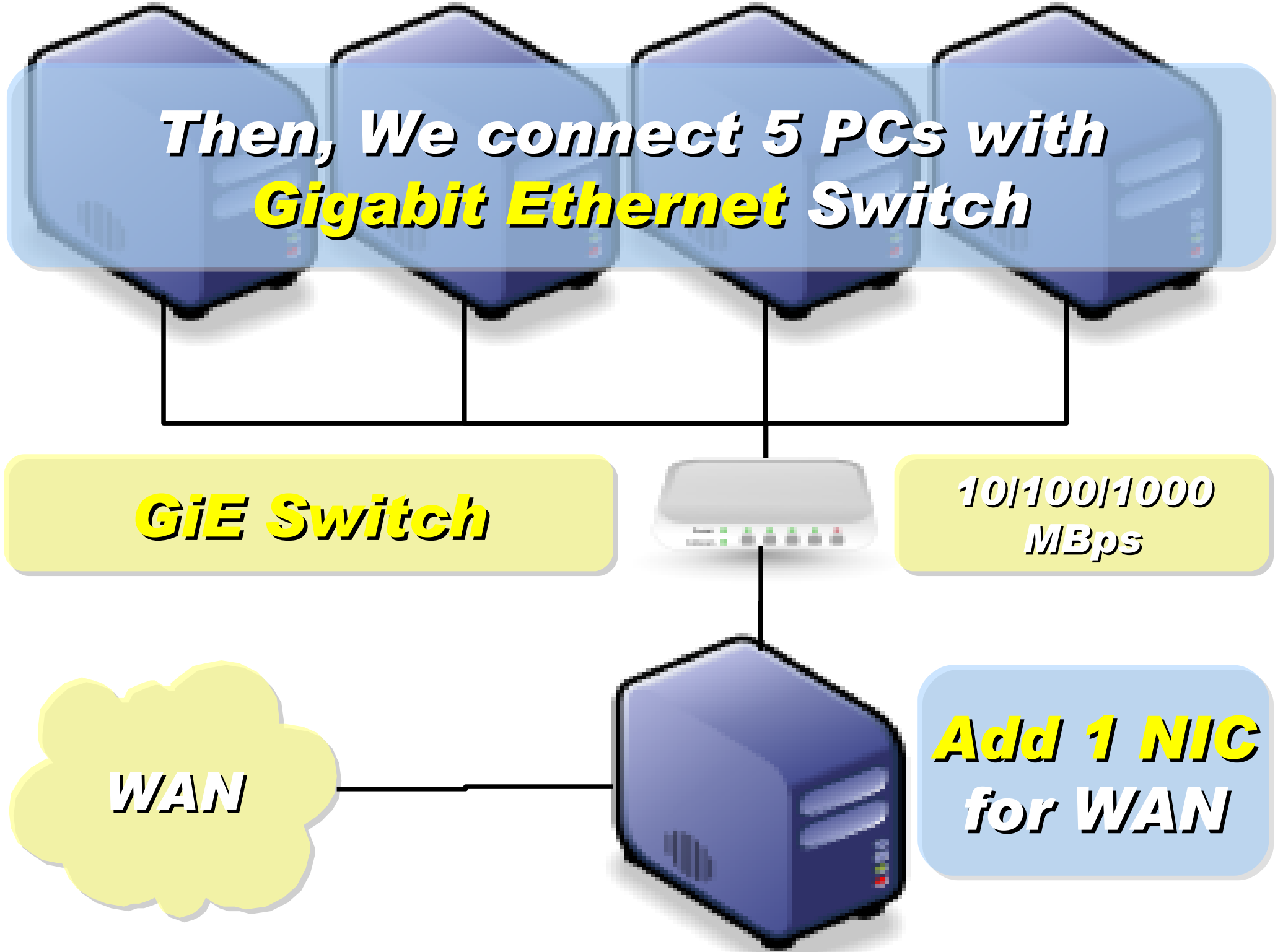
*Then, We connect 5 PCs with
Gigabit Ethernet Switch*

GiE Switch

*10/100/1000
MBps*

WAN

***Add 1 NIC
for WAN***



Compute Nodes

4 Compute Nodes will communicate via LAN Switch. Only Manage Node have Internet Access for Security!

WAN

Manage Node



Compute Nodes

Basic System Setup for Cluster

Messaging

MPICH

GCC

Bash

Perl

Account Mgmt.

SSHD

NIS

YP

GNU Libc



Kernel Module

Linux Kernel

Boot Loader

On **Manage Node**,
We need to install **Scheduler** and
Network File System for sharing
Files with **Compute Node**

Job Mgmt.

OpenPBS

File Sharing

NFS

Extra

Messaging

MPICH

GCC

Bash

Perl

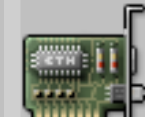
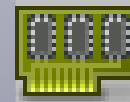
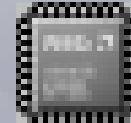
Account Mgmt.

SSHD

NIS

YP

GNU Libc



Kernel Module

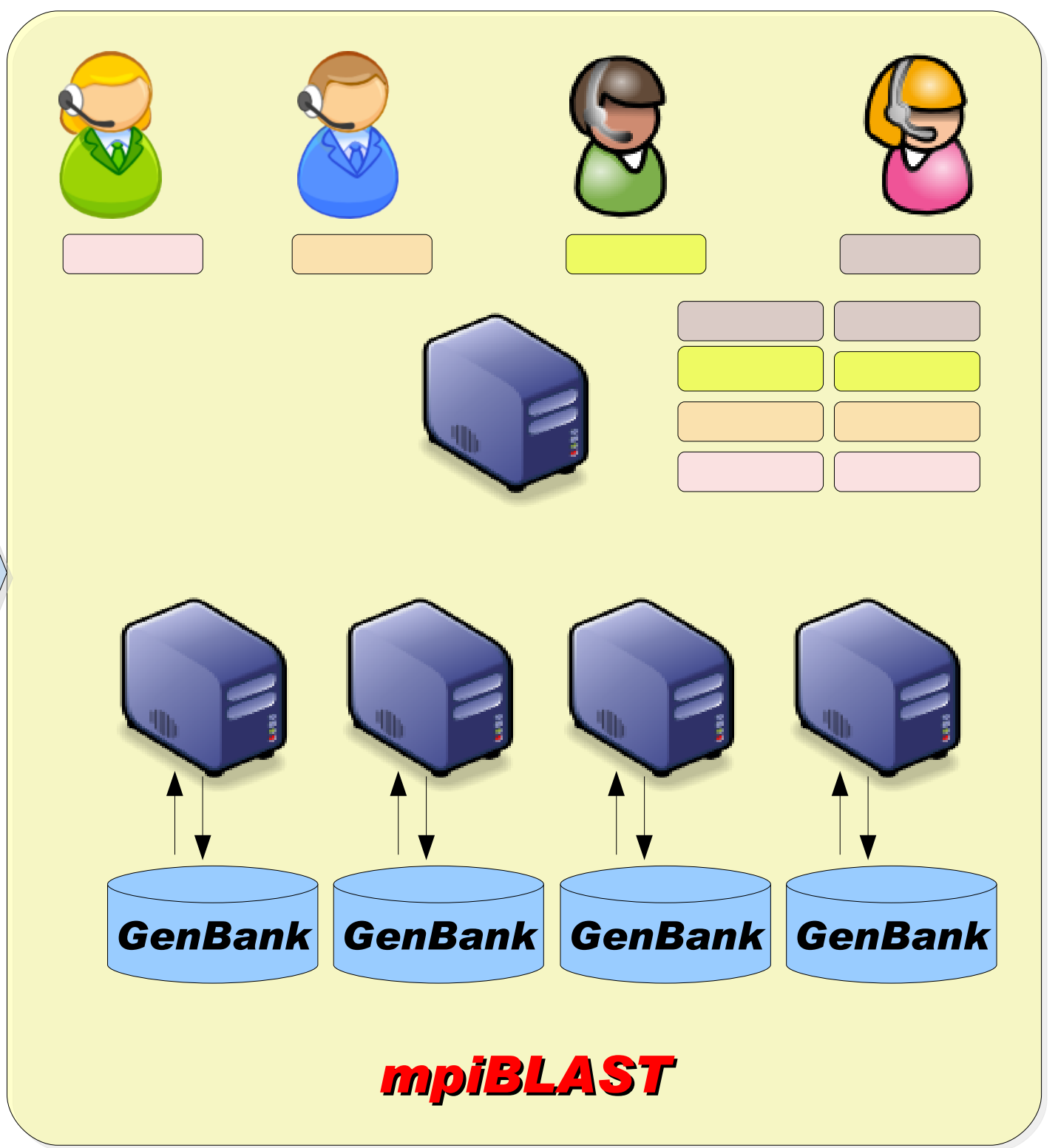
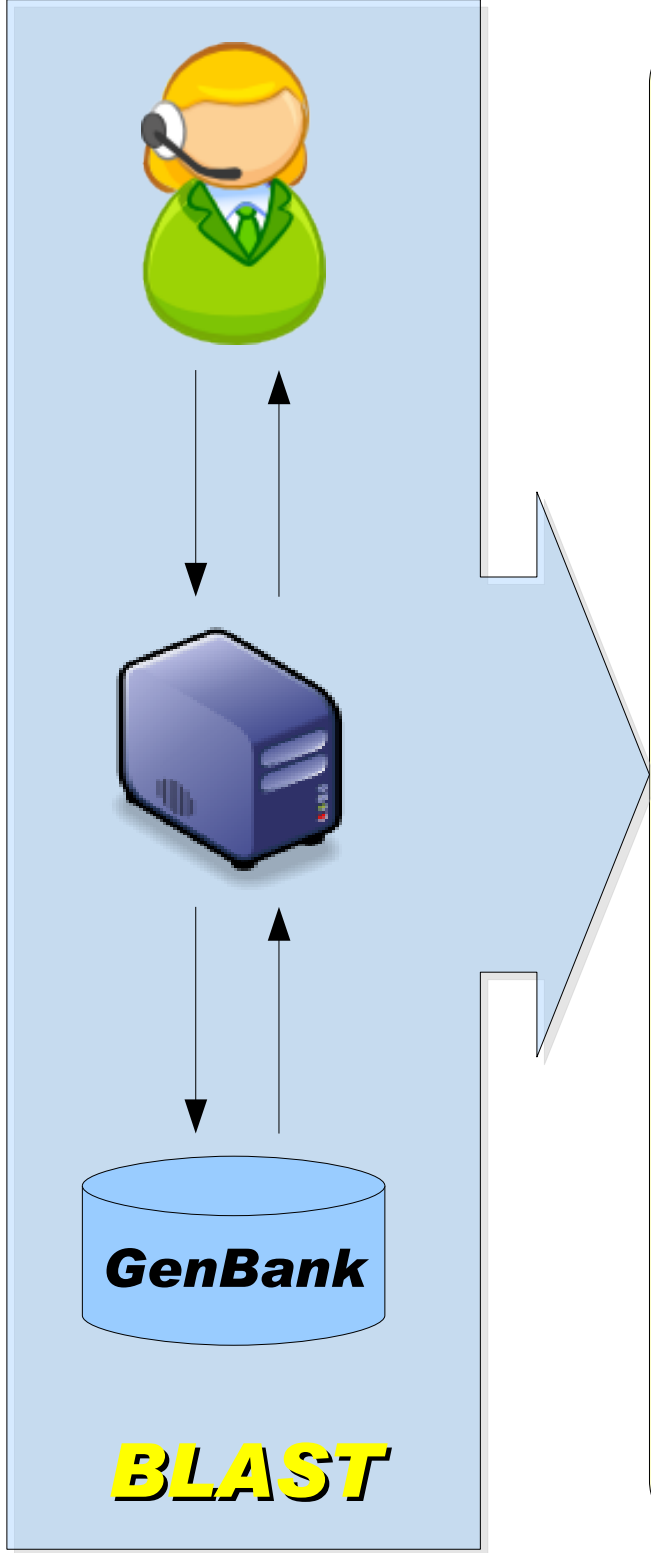
Linux Kernel

Boot Loader

mpiBLAST

- <http://www.mpiblast.org/>
- An open-source, parallel implementation of NCBI BLAST
- 特點：
 - Database fragmentation
 - Query segmentation
 - Parallel input/output
- 設計理念：
 - *The Design, Implementation, and Evaluation of mpiBLAST.*
 - <http://www.mpiblast.org/downloads/pubs/cwce03.pdf>
- 類似工具：
 - TurboWorx TurboBLAST
 - Parallel BLAST by Caltech







PART 2.2 :

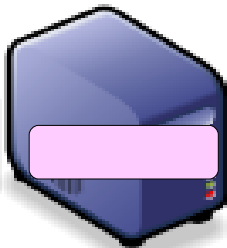
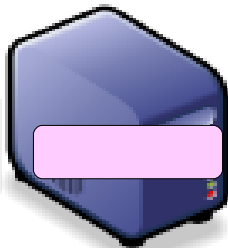
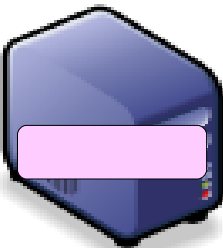
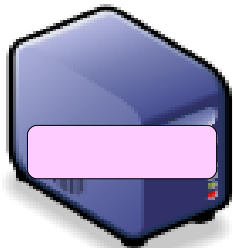
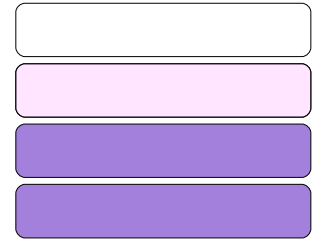
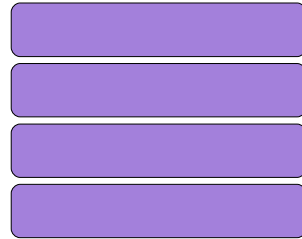
Grid 101 & mpiBLAST-G2

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Grid \approx Cluster of Cluster



mpiBLAST-G2

- ***mpiBLAST-G2 is an enhanced parallel program of LANL's mpiBLAST. It is based on [Globus Toolkit 2.x](#) and [MPICH-g2](#).***
- ***Bioinformatics Technology and Service (BITS) team of [Academia Sinica Computing Centre \(ASCC\), Taiwan](#)***
- 參考：
 - ***The MPIBLAST-g2 Introduction***
 - ***MPIBLAST-g2 Example***
 - ***mpiBlast-G2 with GT4***



中央研究院計算中心



PART 2.3 :

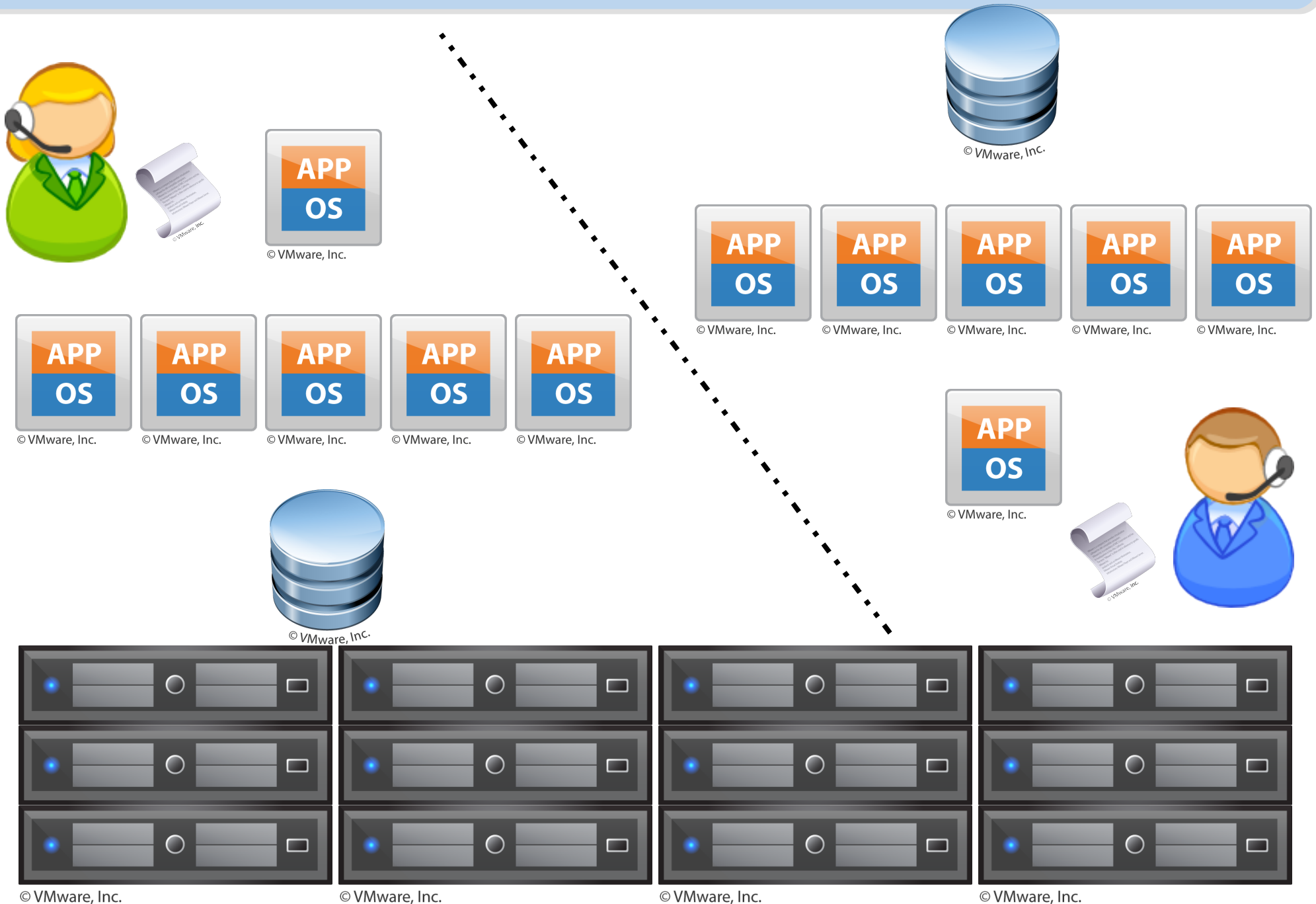
Cloud 101 & CloudBLAST

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Powered by **DRBL**

Cloud \approx Virtualization + Cluster



RunBLAST : mpiBLAST in Amazon EC2

The screenshot shows the RunBlast.com web interface. At the top, there are input fields for 'AWS Access Key' (containing '054F2VTX3A67EW2MG802') and 'AWS Secret Key' (masked with asterisks). Below these are buttons for 'Add Machine', 'Refresh Table', 'Stop All', 'Reset Login Keys', and 'About'. A table displays the status of EC2 instances:

	Status	Public Name	Internal Name
1	running	ec2-67-202-36-153.compute-1.amazonaws.com	domU-12-31-38-00-6C-C8.compute-1.internal
2	running	ec2-67-202-24-53.compute-1.amazonaws.com	domU-12-31-38-00-29-B1.compute-1.internal
3	running	ec2-72-44-46-12.z-2.compute-1.amazonaws.com	domU-12-31-35-00-35-12.z-2.compute-1.internal
4	running	ec2-72-44-47-251.z-2.compute-1.amazonaws.com	domU-12-31-35-00-40-71.z-2.compute-1.internal
5			
6			

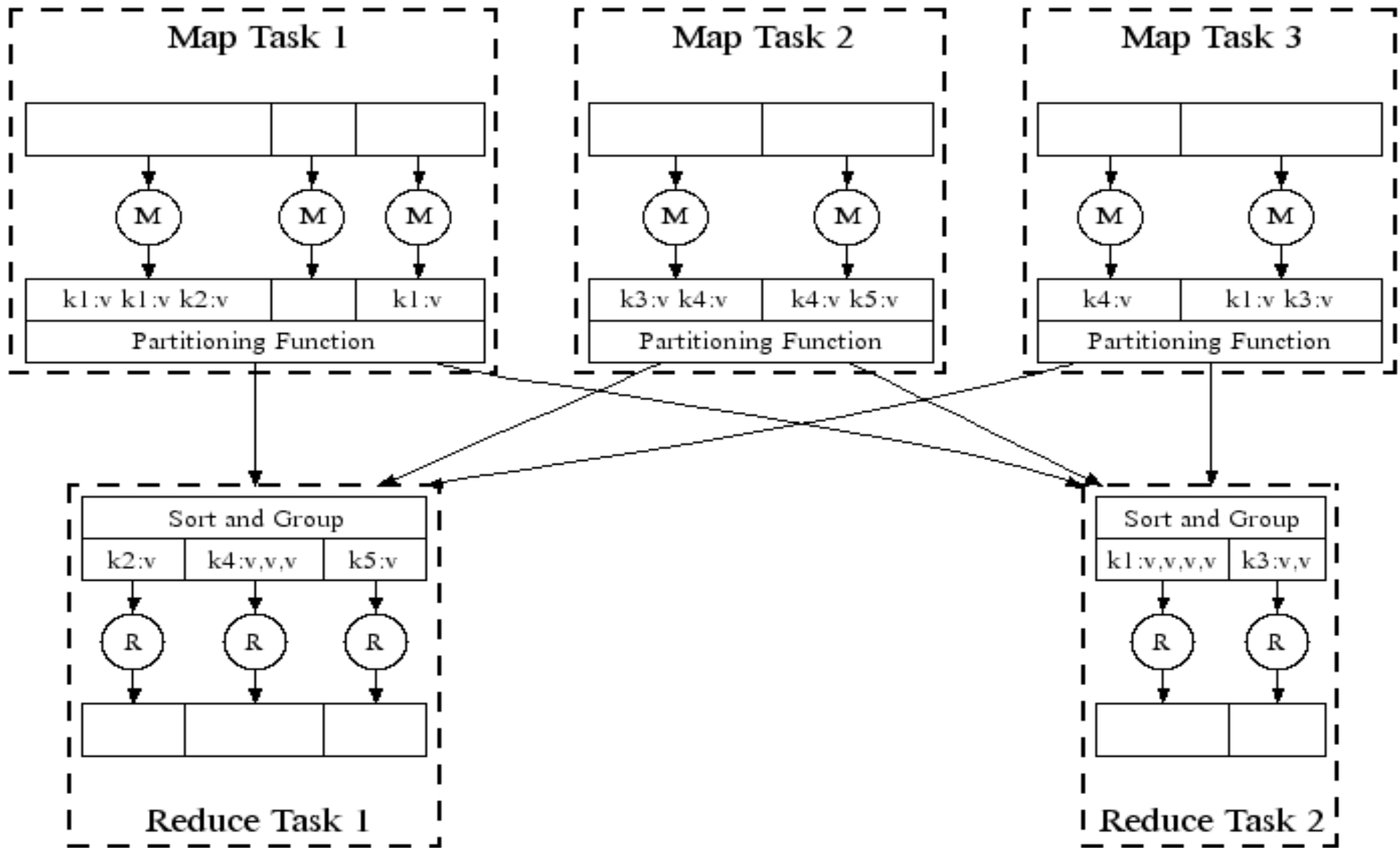
Below the table, a progress bar shows 'Worker Threads: 0'. A log window at the bottom displays the following text:

```
machines status table updated  
machines status table updated  
machines status table updated  
machines status table updated  
machines status table updated  
machines status table updated  
machines status table updated  
machines status table updated  
machines status table updated  
machines status table updated
```

The video player interface at the bottom shows a progress bar and a timestamp of 00:18 / 06:13.

Video: <http://www.runblast.com/videos/runblast-blastwizard.swf>

Map/Reduce



CloudBLAST

- “**CloudBLAST: Combining MapReduce and Virtualization on Distributed Resources for Bioinformatics Applications**”, eScience 2008
- 特點：採用 **MapReduce** 演算法進行 **BLAST** 運算

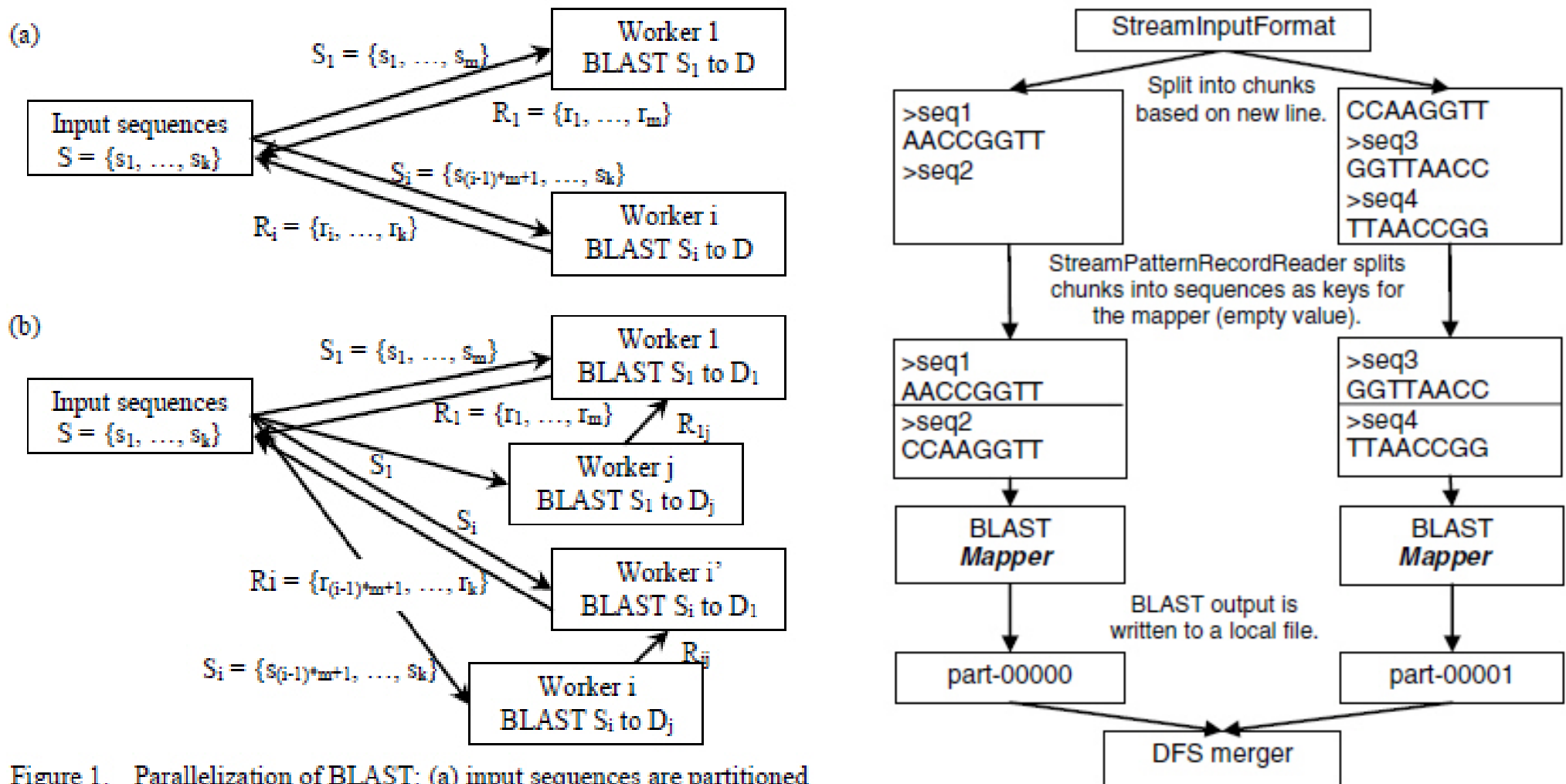


Figure 1. Parallelization of BLAST: (a) input sequences are partitioned



PART 3 :

Open Source for Bioinformatics

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自由軟體 (Free Software)

站在巨人的肩膀上，是自由軟體發展的理念。其靈活、可自由複製、分享的價值，將有效解決資訊教育的管理成本及商業軟體高成本負擔的問題。



Open Source is your Friend !!

- Open Bioinformatics Foundation - <http://www.bioinformatics.org>
 - BioPerl - <http://bio.perl.org>
 - BioPython - <http://biopython.org>
 - BioPHP - <http://biophp.org>
 - BioJava - <http://biojava.org>
- C++ Bio Sequence Library
 - <http://libseq.sourceforge.net/>
 - C++ 版本的序列分析函式庫
- Bio-SPICE - <http://biospice.sourceforge.net/>
- BioEra - <http://bioera.net/>
 - 跟腦科學有蠻強的關聯性，主要功能是在做訊號處理。
- NCBI Viewer - <http://ncbiviewer.bravehost.com/>

Conclusion

***HOW BIG
CAN YOU
THINK ??***

高速計算的工具很多，困難的是**找個好題目**！！



Questions?

Slides - <http://trac.nchc.org.tw/cloud>

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Powered by DRBL

Research topics about PC Cluster

