

Title: 14/15 PSI - Mathematica

Date: Sep 05, 2014 10:30 AM

URL: <http://pirsa.org/14090040>

Abstract:

Multi-Tiered Strategy

- Tier 1: Personal Devices
 - Laptop, desktop
- Tier 2: Scientific Computing Environment (SCE)
 - Shared workstations with remote access
 - Virtual machines
- Tier 3: High Performance Computing (HPC)
 - HPC system “Titan”, access via batch queue
- Tier 4: Support for using outside resources
 - Sharcnet, Scinet, XSEDE, ...

Research Technologies

- Liaison between IT support group and researchers
- Consulting and support e.g. for:
 - Questions on Latex, Mathematica, ...
 - Particular software package
 - Assistance with programming (C, C++, Fortran, Python, Perl, ...)
 - Consulting on numerical algorithms
 - Collaboration on projects/publications
- consult@perimeterinstitute.ca,
or office 350 (new wing, next to elevator)

Scientific Computing Environment

- 7 “regular” Linux workstations, located in a server room
- Names: compute, compute1, ..., compute6
- Running Ubuntu, with many additional packages installed
 - 8 Intel cores with 2.4 GHz
 - 40 GByte RAM
 - Using Perimeter home directory
- Also 1 GPU workstation named “Nvidia”, same software, has Nvidia GPU
- Access via ssh:
 - Login: ssh yourlogin@compute.pi.local
 - Copy files: access via network drive
- Mathematica: can use remote desktop

```
Terminal Shell Edit View Window Help 100% Fri Sep 5 10:45 Erik Schnetter
eschnett — 88x31
bash
Last login: Fri Sep 5 10:26:35 on ttys018

* keychain 2.7.1 ~ http://www.funtoo.org
* Found existing ssh-agent: 390
* Found existing gpg-agent: 438
* Known ssh key: /Users/eschnett/.ssh/id_dsa

eschnett@Redshift:~ (10:43:36)
$ ssh eschnetter@compute@pi.local
```

```
Terminal Shell Edit View Window Help 100% Fri Sep 5 10:52 Erik Schnetter
ssh
Welcome to Ubuntu 14.04.1 LTS (GNU/Linux 3.13.0-34-generic x86_64)

* Documentation:  https://help.ubuntu.com/

System information as of Fri Sep  5 10:50:26 EDT 2014

System load:  0.25          Processes:            402
Usage of /:   81.7% of 94.26GB Users logged in:      9
Memory usage: 8%          IP address for em1:  10.10.153.109
Swap usage:   0%          IP address for virbr0: 192.168.122.1

Graph this data and manage this system at:
  https://landscape.canonical.com/

*** System restart required ***
Last login: Fri Sep  5 10:19:03 2014 from 10.10.164.141
eschnetter@compute:~ (10:50:56)
$ ls
bin          Desktop     Downloads  intel      mars       Pictures    share       Templates
canopy      dist       Enthought  lib        Music      Public      spaces-project Videos
compute    Documents  etc        libexec    oldhome    public_html src         web_dev
eschnetter@compute:~ (10:51:02)
$ math
Mathematica 9.0 for Linux x86 (64-bit)
Copyright 1988-2013 Wolfram Research, Inc.

In[1]:= 2+3

Out[1]= 5

In[2]:= █
```

```
Terminal Shell Edit View Window Help 100% Fri Sep 5 10:54 Erik Schnetter
ssh

In[1]:= 2+3

Out[1]= 5

In[2]:= eschnetter@compute:~ (10:52:28)
$ logout
Connection to compute.pi.local closed.
eschnett@Redshift:~ (10:52:53)
$ ssh eschnetter@nvidia.pi.local
Welcome to Ubuntu 14.04.1 LTS (GNU/Linux 3.13.0-34-generic x86_64)

* Documentation:  https://help.ubuntu.com/

System information as of Fri Sep  5 10:19:28 EDT 2014

System load:  3.05                Processes:            422
Usage of /:   69.1% of 110.61GB   Users logged in:    1
Memory usage: 15%                IP address for em1: 10.10.153.105
Swap usage:   3%                 IP address for virbr0: 192.168.122.1

Graph this data and manage this system at:
https://landscape.canonical.com/

*** System restart required ***
Last login: Fri Sep  5 10:19:08 2014 from 10.10.164.141
eschnetter@nvidia:~ (10:52:57)
$ export DISPLAY=:247
eschnetter@nvidia:~ (10:53:10)
$ Mathematica
█
```

Scientific Computing Environment

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 - Copy files: access via network drive
- Mathematica: can use remote desktop

Software Packages on SCE

- Mathematica, Maple, Matlab, Magma, Sage, Ipython, ...
- Python, Perl
- GNU C, C++, Fortran
- CUDA, OpenCL
- Intel compilers (C, C++, Fortran, MKL, debugger/profiler)
- RNPL
- gnuplot
- SuperMongo
- DataVault
- VisIt (visualisation)
- Many more – ask if you need something

Chrome File Edit View History Bookmarks Window Help 100% Fri Sep 5 10:59 Erik Schnetter

localhost:8888/notebooks/Untitled2.ipynb

IP[y]: Notebook Untitled2 (unsaved changes)

File Edit View Insert Cell Kernel Help

Code Cell Toolbar: None

```
In [ ]: 2+
```

Chrome File Edit View History Bookmarks Window Help 100% Fri Sep 5 11:00 Erik Schnetter

localhost:8888/notebooks/Untitled2.ipynb

IP[y]: Notebook Untitled2 (unsaved changes)

File Edit View Insert Cell Kernel Help

Code Cell Toolbar: None

```
In [1]: 2+3
Out[1]: 5

In [2]: x=5
In [3]: x+1
Out[3]: 6

In [4]: solve(x+1==0,x)

-----
NameError                                Traceback (most recent call last)
<ipython-input-4-f44186fc3f32> in <module>()
----> 1 solve(x+1==0,x)

NameError: name 'solve' is not defined

In [ ]: import * from sympy
```

Chrome File Edit View History Bookmarks Window Help 100% Fri Sep 5 11:00 Erik Schnetter

localhost:8888/notebooks/Untitled2.ipynb

IP[y]: Notebook Untitled2 (unsaved changes)

File Edit View Insert Cell Kernel Help

Code Cell Toolbar: None

```
In [3]: x+1
Out[3]: 6

In [4]: solve(x+1==0,x)

-----
NameError                                Traceback (most recent call last)
<ipython-input-4-f44186fc3f32> in <module>()
----> 1 solve(x+1==0,x)

NameError: name 'solve' is not defined

In [5]: import * from sympy

File "<ipython-input-5-97d2f4f0dbf0>", line 1
import * from sympy
      ^
SyntaxError: invalid syntax

In [ ]:
```

Chrome File Edit View History Bookmarks Window Help 100% Fri Sep 5 11:01 Erik Schnetter

localhost:8888/notebooks/Untitled2.ipynb

IP[y]: Notebook Untitled2 (unsaved changes)

File Edit View Insert Cell Kernel Help

Code Cell Toolbar: None

Out[3]:

In [4]: `solve(x+1==0,x)`

```
-----  
NameError                                Traceback (most recent call last)  
<ipython-input-4-f44186fc3f32> in <module>()  
----> 1 solve(x+1==0,x)  
  
NameError: name 'solve' is not defined
```

In [6]: `import sympy`

In [8]: `sympy.vars("x y z")`

```
-----  
AttributeError                            Traceback (most recent call last)  
<ipython-input-8-8dfc717a604d> in <module>()  
----> 1 sympy.vars("x y z")  
  
AttributeError: 'module' object has no attribute 'vars'
```

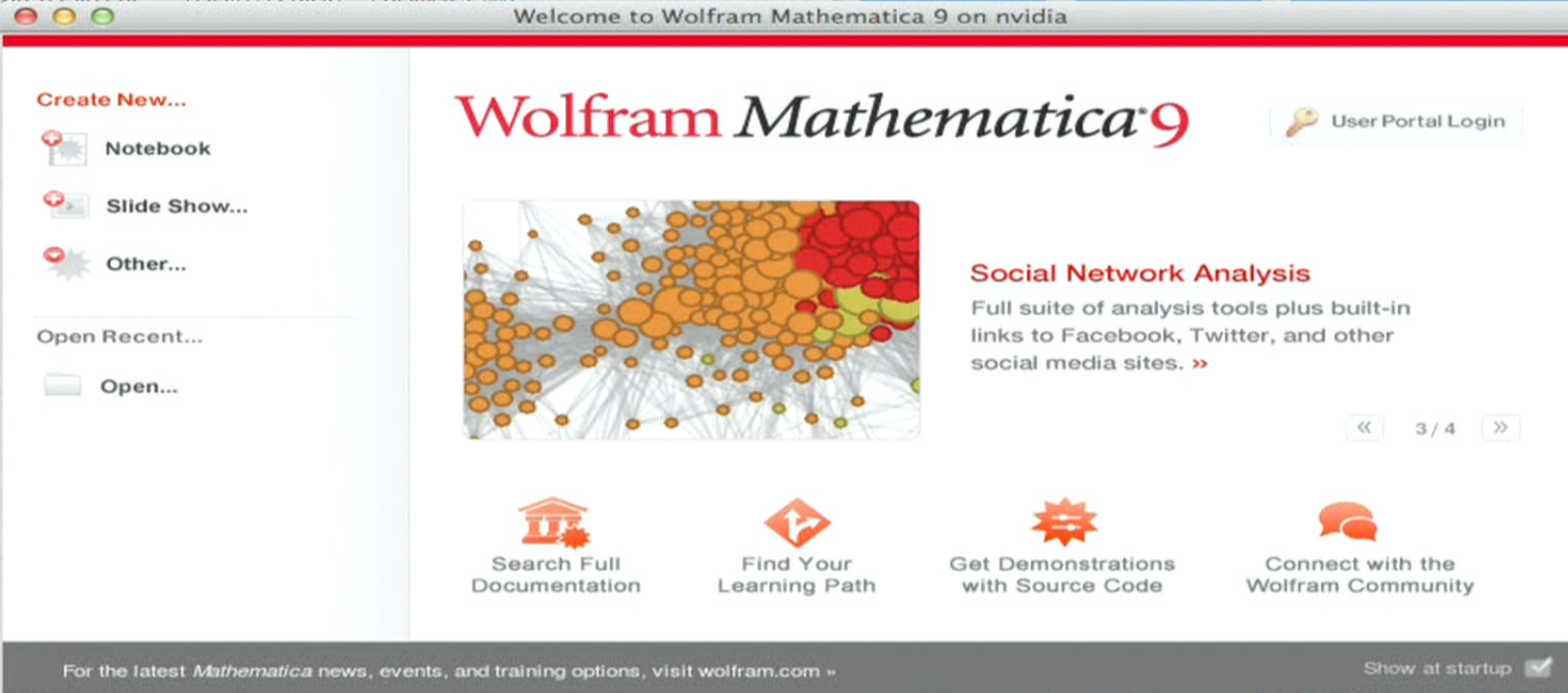
In []:

Xpra Info Features Encoding Actions 100% Fri Sep 5 11:02 Erik Schnetter

```

eschnett — x — 80x53
2014-09-05 10:57:14,711 sending updated screen size to server: 1024x768 with 1 s
creens
2014-09-05 10:57:14,712 'redshift.local' (361x270 mm)
2014-09-05 10:57:14,712 monitor 1
2014-09-05 10:57:30,710 sending updated screen size to server: 2944x1200 with 1
creens
2014-09-05 10:57:30,710 'redshift.local' (1030x423 mm)
Welcome to Wolfram Mathematica 9 on nvidia
Create New...
Notebook
Slide Show...
Other...
Open Recent...
Open...
(Xpra:95 fact it is
(Xpra:95 ct it is of
(Xpra:95 fact it is
(Xpra:95 act it is o
2014-09-05
2014-09-05 VBO, numpy_
2014-09-05
2014-09-05
2014-09-05
2014-09-05 11:02:08,903 monitor 1
2014-09-05 11:02:13,670 server: Linux Ubuntu 14.04 trusty, Xpra version 0.12.3 (
r6875)
2014-09-05 11:02:13,680 Attached to ssh/eschnetter@nvidia.pi.local/247 (press Co
ntrol-C to detach)
2014-09-05 11:02:13,730 Unable to load nones_formathandler accelerator from Open
GL_accelerate

```



Welcome to Wolfram Mathematica 9 on nvidia

Wolfram Mathematica[®] 9

[User Portal Login](#)

Social Network Analysis
 Full suite of analysis tools plus built-in links to Facebook, Twitter, and other social media sites. >>

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Show at startup

Mac OS Xpra window titled "Untitled-1 * on nvidia". The menu bar includes File, Edit, Insert, Format, Cell, Graphics, Evaluation, Palettes, Window, and Help. The system status bar shows the date and time as "Fri Sep 5 11:03" and the user as "Erik Schnetter".

The notebook interface shows the following input and output:

```
In[1]:= 2 + 3
Out[1]= 5

In[2]:= SystemInformation[]
```

The output of `SystemInformation[]` is displayed in a structured view with the following sections:

- Kernel**: Kernel Count 0, Running Kernels {}, Kernel Configuration (<<24 local kernels>>)
- Parallel**: Processor Count 24
- Devices**: Debugging True, Automatic Launching Automatic, Failed Kernel Relaunching True, Evaluation Failure Recovery Retry
- Network**: Shared Resources, Connection Methods
- Parallel Tools Version 8.0

A "Copy" button is located below the output. At the bottom of the notebook, there is a "get data rules" button and a search icon.

Xpra Info Features Encoding Actions 100% Fri Sep 5 11:03 Erik Schnetter

Untitled-1 * on nvidia

File Edit Insert Format Cell Graphics Evaluation Palettes Window Help

In[1]:= 2 + 3
Out[1]= 5

In[2]:= SystemInformation[]

Kernel	Front End	Links	Parallel	Devices	Network
Version	9.0 for Linux x86 (64-bit) (February 7, 2013)				
Release ID	9.0.1.0 (4092720, 4092445)				
Patch Level	0				
Activation Key	3006-1939-HPEX6R				
Machine ID	6501-45792-10754				
User Name	eschnetter				
Machine Name	nvidia				
Machine Domains	()				
License Server	mathm.pi.local				
Max License Processes	∞				
License Expiration Date	Thu 24 Sep 2015 00:00:00				
Machine Type	PC				
Operating System	Unix				
Processor Type	x86-64				
Language	English				
Character Encoding	UTF-8				
System Character Encoding	UTF-8				
Time Zone	-4.				
Creation Date	Thu 7 Feb 2013 21:55:56				
Installation Directory	/usr/local/Wolfram/Mathematica/9.0 >				
Initialization Files Loaded	▶ 5 files				
▶ Directories					
▶ Packages & Files					
▶ Streams					
▶ MathLink					
▶ External Compilers					
▶ Advanced					
Benchmark with <i>MathematicaMark</i> ...					

Out[2]=

100%

Xpra Info Features Encoding Actions 100% Fri Sep 5 11:06 Erik Schnetter

Untitled-1 * on nvidia

File Edit Insert Format Cell Graphics Evaluation Palettes Window Help

Out[2]=

Machine Domains	{}
License Server	mathm.pl.local
Max License Processes	∞
License Expiration Date	Thu 24 Sep 2015 00:00:00
Machine Type	PC
Operating System	Unix
Processor Type	x86-64
Language	English
Character Encoding	UTF-8
System Character Encoding	UTF-8
Time Zone	-4.
Creation Date	Thu 7 Feb 2013 21:55:56
Installation Directory	/usr/local/Wolfram/Mathematica/9.0 >
Initialization Files Loaded	▶ 5 files

- ▶ Directories
- ▶ Packages & Files
- ▶ Streams
- ▶ MathLink
- ▶ External Compilers
- ▶ Advanced

Benchmark with *MathematicaMark* ...

Copy

In[3]:= `$ProcessID`

Out[3]= 5898

`Table[$ProcessID, {i, 4}]`

100%

Xpra Info Features Encoding Actions 100% Fri Sep 5 11:06 Erik Schnetter

Untitled-1 * on nvidia

File Edit Insert Format Cell Graphics Evaluation Palettes Window Help

License Expiration Date Thu 24 Sep 2015 00:00:00

Machine Type PC
Operating System Unix
Processor Type x86-64

Language English
Character Encoding UTF-8
System Character Encoding UTF-8
Time Zone -4.

Creation Date Thu 7 Feb 2013 21:55:56
Installation Directory /usr/local/Wolfram/Mathematica/9.0 >>
Initialization Files Loaded ▶ 5 files

▶ Directories
▶ Packages & Files
▶ Streams
▶ MathLink
▶ External Compilers
▶ Advanced

Benchmark with *MathematicaMark* ...

Copy

Out[2]=

In[3]:= `$ProcessID`

Out[3]= 5898

In[4]:= `Table[$ProcessID, {i, 4}]`

Out[4]= {5898, 5898, 5898, 5898}

`ParallelTable[$ProcessID, {i, 4}]`

100%

Xpra Info Features Encoding Actions 100% Fri Sep 5 11:07 Erik Schnetter

Untitled-1 * on nvidia

File Edit Insert Format Cell Graphics Evaluation Palettes Window Help

License Expiration Date Thu 24 Sep 2015 00:00:00

Machine Type PC
Operating System Unix
Processor Type x86-64

Language English
Character Encoding UTF-8
System Character Encoding UTF-8
Time Zone -4.

Creation Date Thu 7 Feb 2013 21:55:56
Installation Directory /usr/local/Wolfram/Mathematica/9.0 >>
Initialization Files Loaded ▶ 5 files

▶ Directories
▶ Packages & Files
▶ Streams
▶ MathLink
▶ External Compilers
▶ Advanced

Benchmark with *MathematicaMark* ...

Copy

Out[2]=

In[3]:= `$ProcessID`

Out[3]= 5898

In[4]:= `Table[$ProcessID, {i, 4}]`

Out[4]= {5898, 5898, 5898, 5898}

In[5]:= `ParallelTable[$ProcessID, {i, 4}]`

Out[5]= {21918, 21480, 21049, 20618}

100%

Xpra Info Features Encoding Actions 100% Fri Sep 5 11:08 Erik Schnetter

Untitled-1 * on nvidia

File Edit Insert Format Cell Graphics Evaluation Palettes Window Help

License Expiration Date Thu 24 Sep 2015 00:00:00

Machine Type PC
Operating System Unix
Processor Type x86-64

Language English
Character Encoding UTF-8
System Character Encoding UTF-8
Time Zone -4.

Creation Date Thu 7 Feb 2013 21:55:56
Installation Directory /usr/local/Wolfram/Mathematica/9.0 >>
Initialization Files Loaded ▶ 5 files

▶ Directories
▶ Packages & Files
▶ Streams
▶ MathLink
▶ External Compilers
▶ Advanced

Benchmark with *MathematicaMark* ...

Copy

In[3]:= `$ProcessID`
Out[3]= 5898

In[4]:= `Table[$ProcessID, {i, 4}]`
Out[4]= {5898, 5898, 5898, 5898}

In[7]:= `ParallelTable[$ProcessID, {i, 25}]`
Out[7]= {21918, 21918, 21480, 21049, 20618, 20175, 19744, 19305, 18873, 18442, 18002, 17558, 17115, 16682, 16249, 15811, 15381, 14878, 14445, 13976, 13544, 13112, 12670, 12240, 11800}

total plot points histogram length more...

100%

Mac OS Xpra window titled "Untitled-1 * on nvidia". The menu bar includes File, Edit, Insert, Format, Cell, Graphics, Evaluation, Palettes, Window, and Help. The system status bar shows the date and time as "Fri Sep 5 11:10" and the user as "Erik Schnetter".

The main content area displays Mathematica output:

```
Character Encoding UTF-8
System Character Encoding UTF-8
Time Zone -4.

Creation Date Thu 7 Feb 2013 21:55:56
Installation Directory /usr/local/Wolfram/Mathematica/9.0 >
Initialization Files Loaded ▶ 5 files

▶ Directories
▶ Packages & Files
▶ Streams
▶ MathLink
▶ External Compilers
▶ Advanced

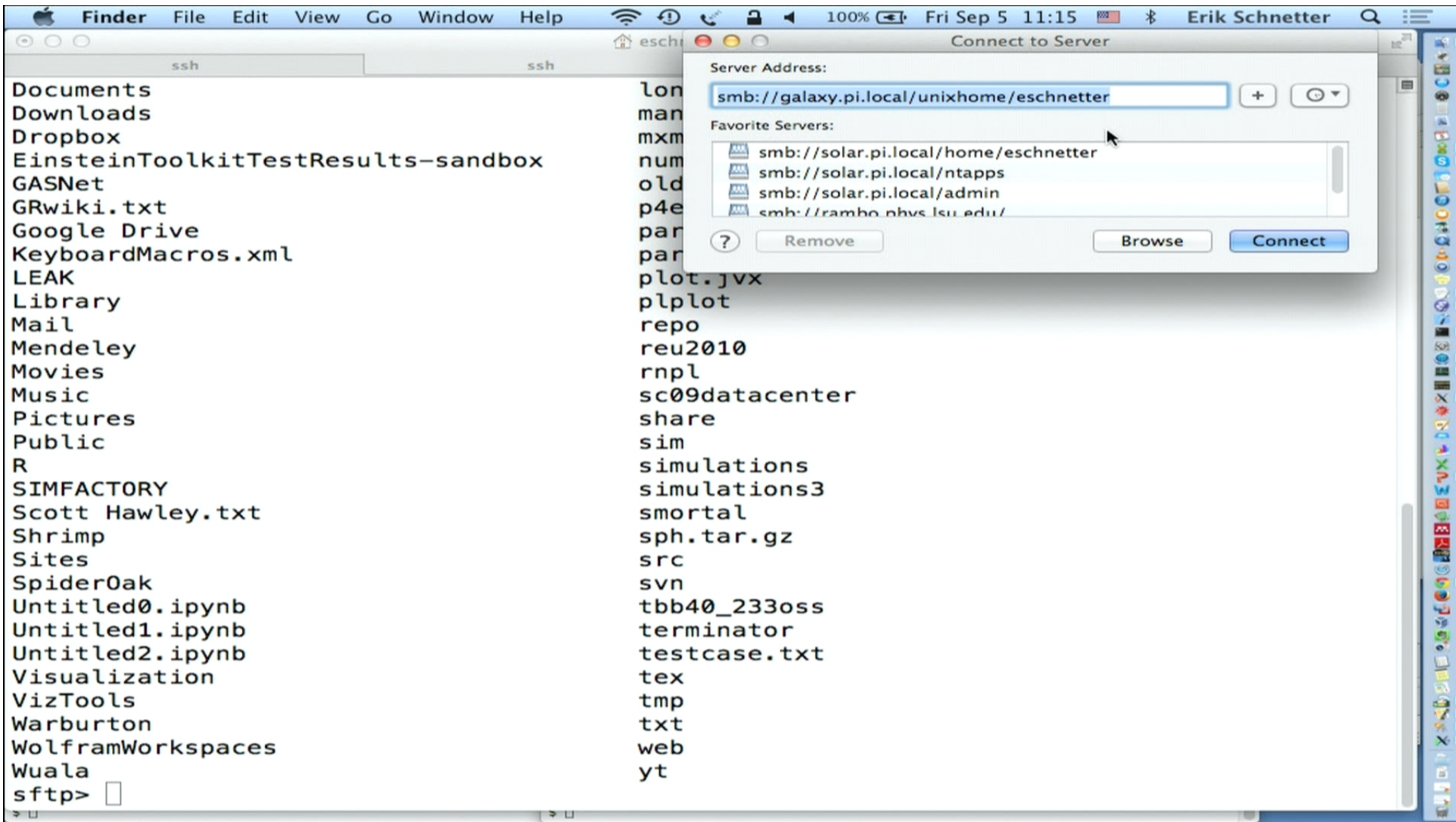
Benchmark with MathematicaMark ...

Copy

In[3]:= $ProcessID
Out[3]= 5898

In[4]:= Table[$ProcessID, {i, 4}]
Out[4]= {5898, 5898, 5898, 5898}

In[7]:= ParallelTable[$ProcessID, {i, 25}]
Out[7]= {21918, 21918, 21480, 21049, 20618, 20175, 19744, 19305, 18873, 18442, 18002, 17558, 17115,
        16682, 16249, 15811, 15381, 14878, 14445, 13976, 13544, 13112, 12670, 12240, 11800}
```



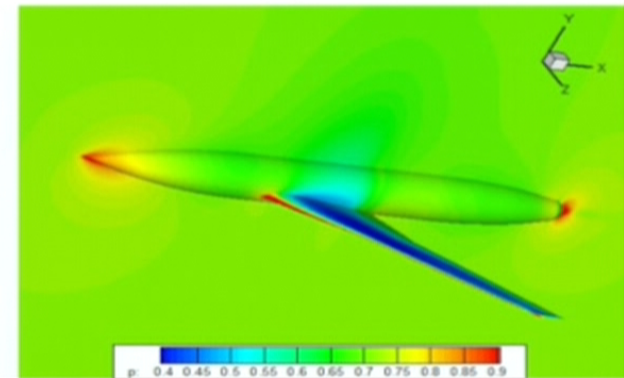
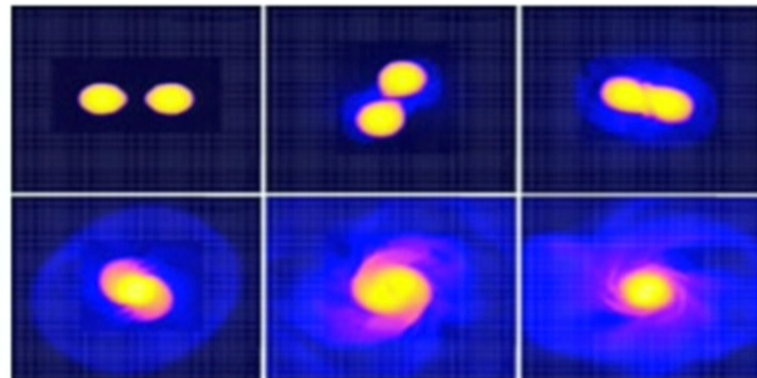
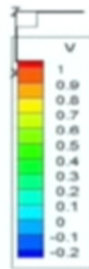
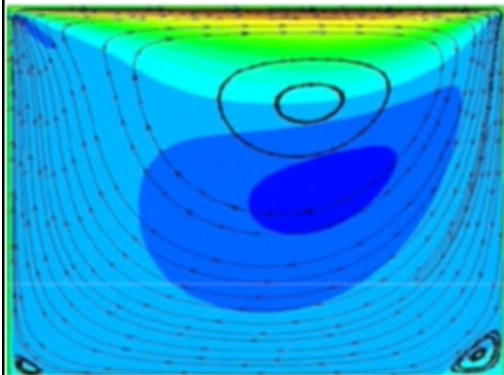
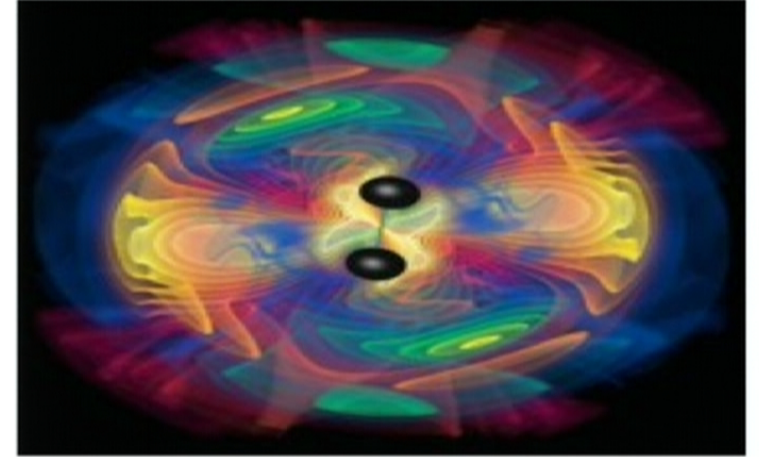
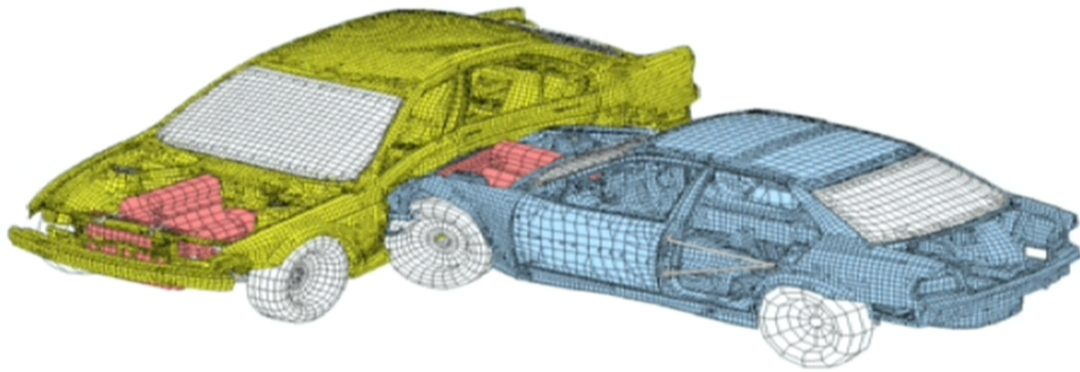
Running Persistent Jobs on SCE

- Persistent job:
 - Add “nohup” when starting a job, e.g. “nohup ./mystuff &”
- Persistent terminal:
 - Use ssh to log in, then use “screen” to start a permanent session:
 - ssh [yourlogin@compute.pi.local](#)
 - screen [may need to wait a minute]
 - ./mystuff
 - Will continue to run if connection is lost. To re-connect, log in again, then
 - screen -r
- Mathematica:
 - Write .m script, run it via “math”, then see above
 - Use e.g. Xpra for a remote desktop

Introduction to Simulation Science

Erik Schnetter, Perimeter Institute
2014-09-05

Simulations



Why Use Simulations?

- Flame propagation in combustion engine: *understand* behaviour that is too fast or too small
- Hurricane modelling: *predict* behaviour
- Car crash testing: *engineer* better devices
- Video games: *create* a fantasy world similar to the real one

**Laws of Physics
(or Chemistry, Biology, ...)**

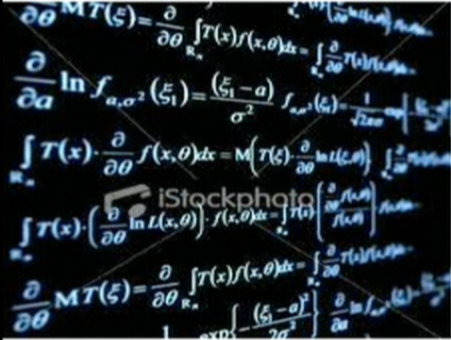


Simulation

**Laws of Physics
(or Chemistry, Biology, ...)**



Simulation



- The physics that is to be simulated is expressed in “the language of Mathematics”
- Called *Scientific Computing* or *Numerical Analysis*

- The resulting systems of equations are solved on large computers
- Called *Supercomputers* because they are as large and awkward as a supertanker

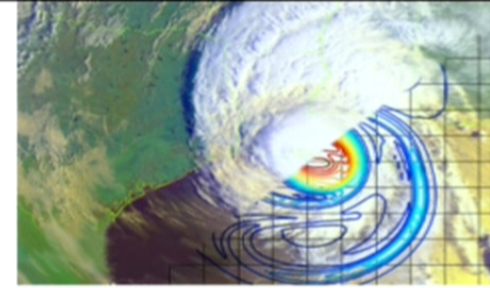


Systems and Equations

- The state of a system is described via variables (density, velocity, pressure, etc.)
- Laws of Physics can then often be described via *PDEs* (Partial Differential Equations)
- A PDE describes how a system is *changing* depending on its current *state*



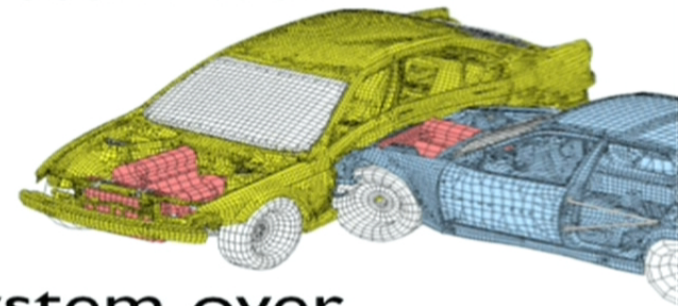
Discretisation



- PDEs describe continuum systems (car body, water, air); these have infinitely many degrees of freedom
- Reduce complexity by approximation via a *discrete system* instead
- Compare e.g. pixels on a TV screen, surface triangulation for visualisation
- Many possibilities:
- finite elements (e.g. small rigid triangles)
- finite volumes (e.g. small cubes)
- finite differences (sample solution on regular grid)
- particles (small chunks of matter)
- many more...

Simulation Procedure

- Choose PDE that describes system well
- Discretise PDE
- Set up initial condition
- Follow each element of the system over many many tiny steps
- A simulation can have billions of elements with millions of steps, taking weeks of computing time



Caveat

- Some systems are described not by PDEs but otherwise (e.g. coupled ODEs, discrete transitions)
- Sometimes not time evolution is interesting, but e.g. equilibrium configuration
- Usually (in real life), PDEs and initial conditions are only *approximations or guesses*, and simulation results *may not be reliable*

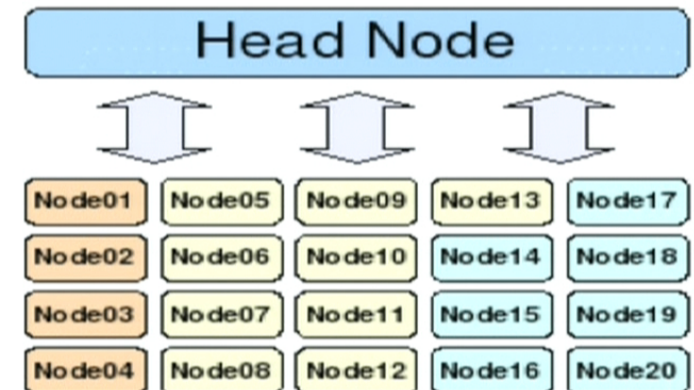


Supercomputer Architectures

Remote Access



- Supercomputers are located in far away places, need to use ssh/gsissh to access
- Log in is to *front end (head node)* only, usually a large workstation
- Cannot (or should not) use front end to run simulations

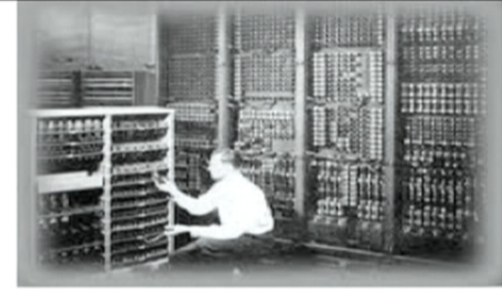


Compute Nodes, Interconnect



- Most supercomputers have a *cluster* architecture with many compute nodes
- Each node has (4 to 32?) cores, similar to a large workstation
- Nodes are connected via a low-latency *communication network* (e.g. Infiniband)
- Overall system has (128 to >8,000?) nodes, or up to 100k cores
- My personal scale:
 - < 1k cores: small,
 - < 10k cores: medium
 - > 10k cores: large

Batch System



- Cannot (or should not) use compute nodes directly
- Need to submit *job* to *batch system*, requesting N nodes...
- ... wait (a few days?) ...
- ... then the job runs
- (... and then one discovers one's errors)
- There is a run time limit, often 24h or 48h
- ... which is inconvenient if one needs to run for 2 weeks: checkpoint/restart
- Batch systems ensure that a supercomputer is not idle; there are always jobs waiting to be executed



TeraGrid™

Allocations



- Need to ensure fair use of supercomputer, prevent individual users from monopolising it
- Typically, an *allocation process* decides who can use how much of a supercomputer's time during a year (similar to writing a grant proposal)
- 1 CPU hour costs about 5 cents
- With this metric, Titan (small HPC system at Perimeter) produces about \$150k worth of CPU time per year

Software

- Installed/available software is system dependent, not just standard Unix systems
- Therefore cannot just install binaries, need to build software manually (or ask administrators to do that)
- HPC developers often prefer command line tools, don't use GUIs (which may not be available)

Software

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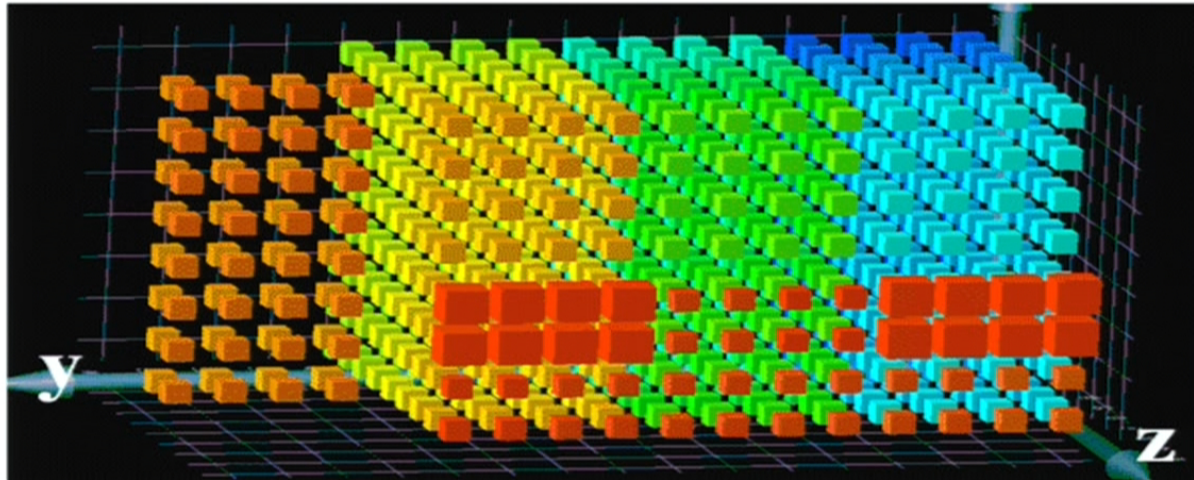
HPC History

- Before MPI: *Vector architectures*, e.g. Cray Y-MP (until ~1992)
- Each instruction acts on 100s or 1000s of data elements “simultaneously” (SIMD)
- Much more efficient than scalar processor (compare conveyor belt vs. hand assembly)
- Disadvantages: too inflexible for dynamic data structures, too expensive due to custom-designed (low-volume) hardware



HPC History, Cont'd

- After vector machines, *cluster architecture* became prevalent (Cray T3D, 1993)
- Basic idea: have many simple nodes, connected by high-speed network
- Nodes need to communicate (*exchange messages*) during computation
- Also called *Beowulf architecture*, esp. if only a cheap network is used



Node connectivity in a Cray T3E

MPI Programming

- Each process runs an independent copy of the program
- Each copy has a unique number assigned to it(0...N-1)
- The program needs to divide the total workload into N pieces, and assign one to each process
- The processes can talk to each other *only* by exchanging messages
- MPI hides low-level, system-dependent communication details from the programmer
- MPI messages are (by default) *ordered* and *reliable*



Examples of Real Life Message Passing

- Message Passing is very common, even in the real world; for example:
 - Letters via the post office
 - Email
 - Phone text messages
 - Newspapers
 - Chinese whispers game
 - Monopoly
- However, these are NOT message passing – they are *streams* or *interactive* instead:
 - Phone conversation
 - Watching TV
 - Google Docs
 - Charades game
 - WoW

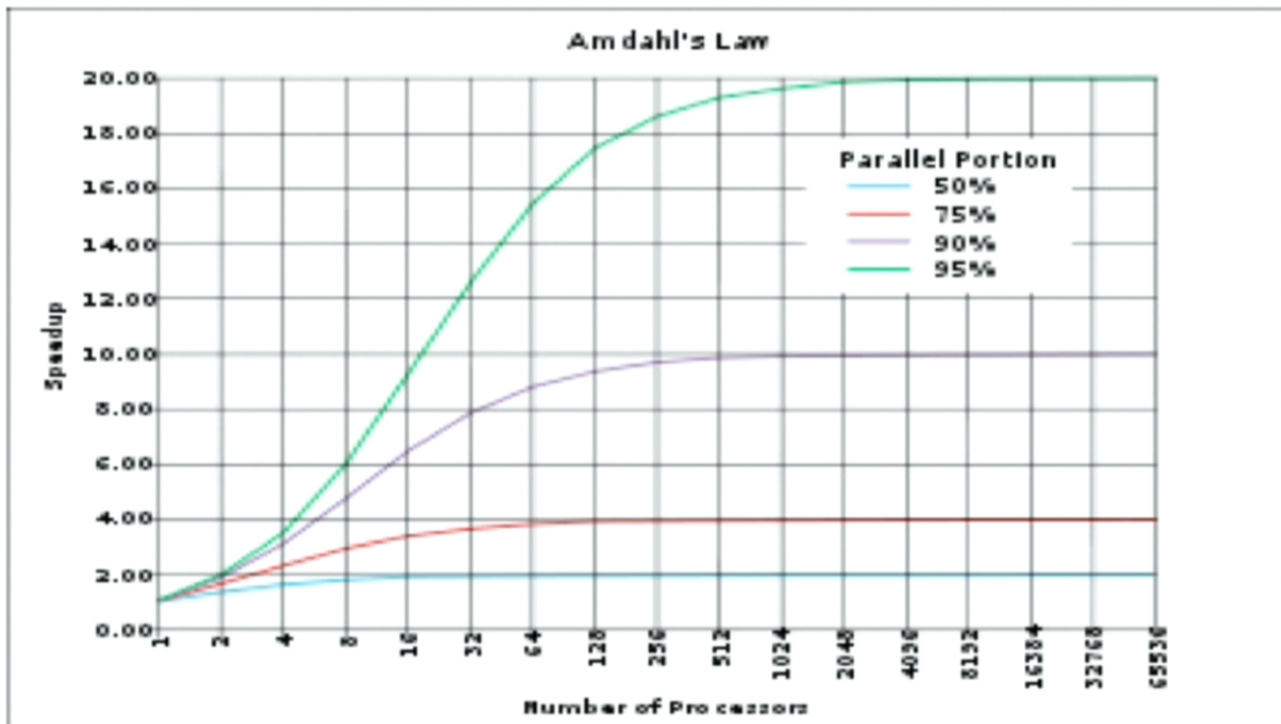
Distributed Array Implementation

- `set-element(n,x)`:
 1. determine which process owns element n
 2. send message to that process containing index n and value x
 3. check whether message has been received
 4. if so, set element n to x
- `x = get-element(n)`:
 1. determine which process owns element n
 2. send message to that process with index n
 3. check whether message has been received
 4. if so, get element n ...
 5. ... and send message back with value x
 6. wait for result

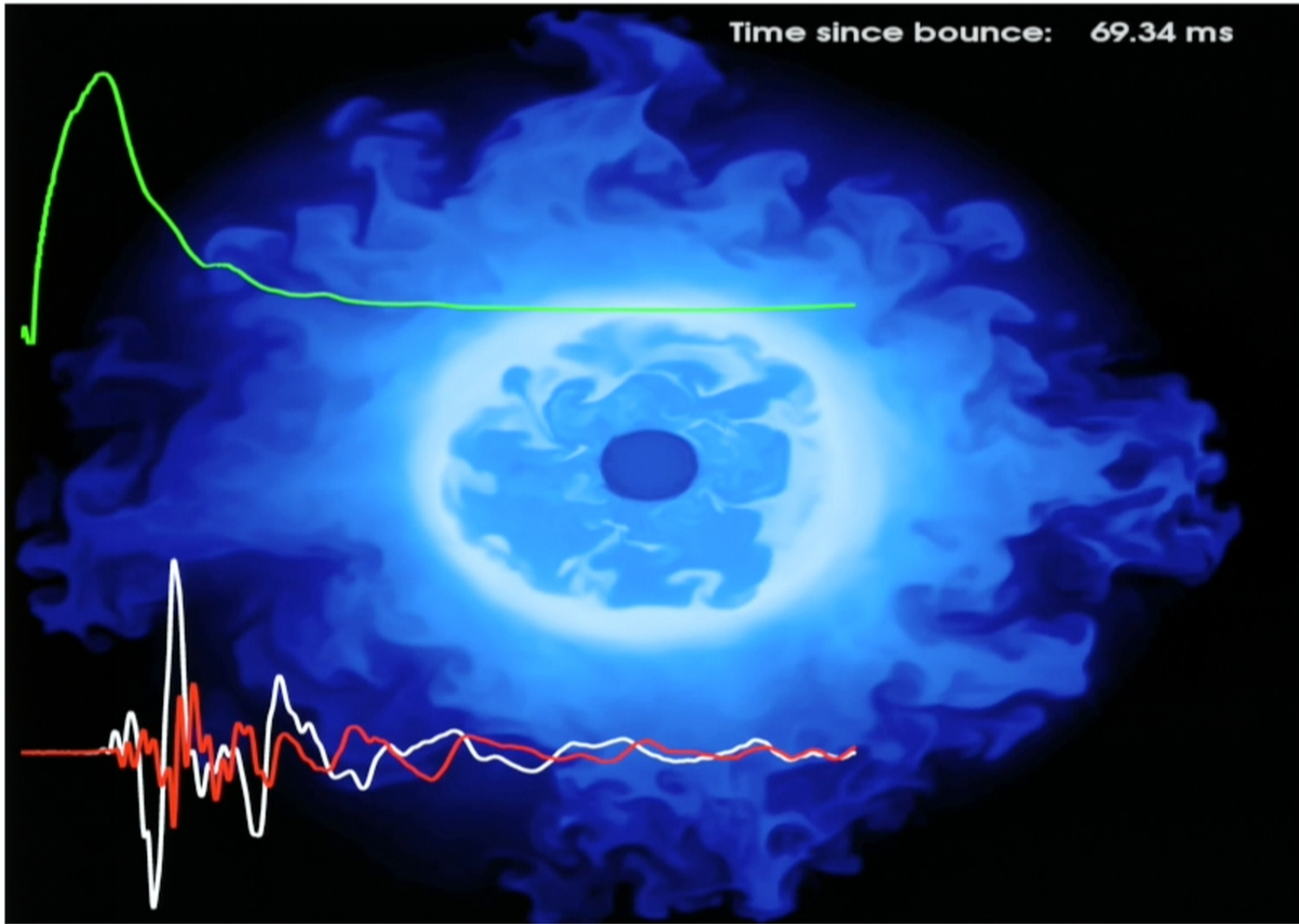
In reality, would not send individual elements, but would send *batches* of elements to reduce latency

Amdahl's Law

- When running on N processes, not necessarily N times as fast – overhead
- Overhead determines maximum possible parallel speedup



100,000-fold speedup requires >99.999% parallelisation



Time Since Big Bang: 7 Billion Years

