High performance computation of relativistic many-body effects in atoms

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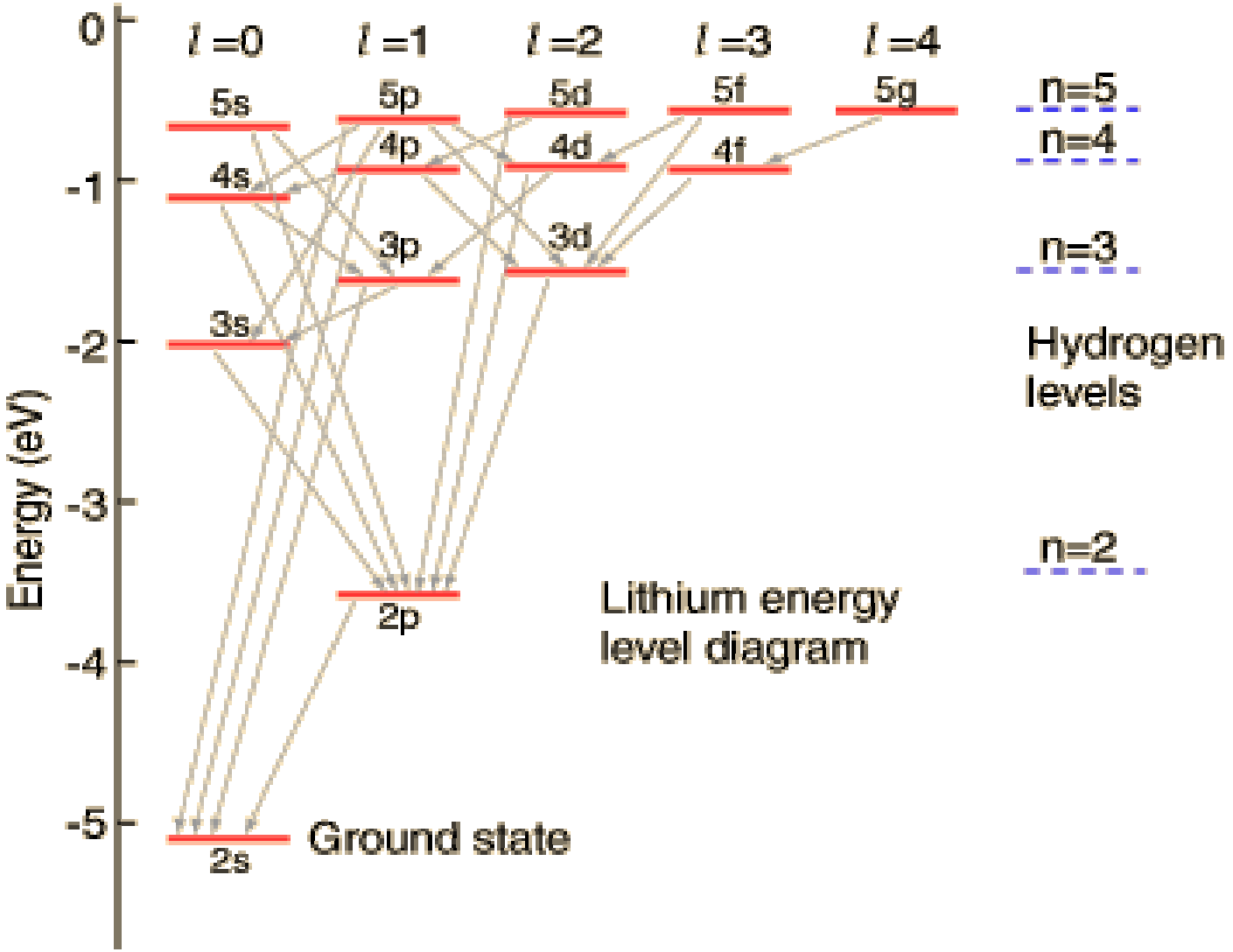
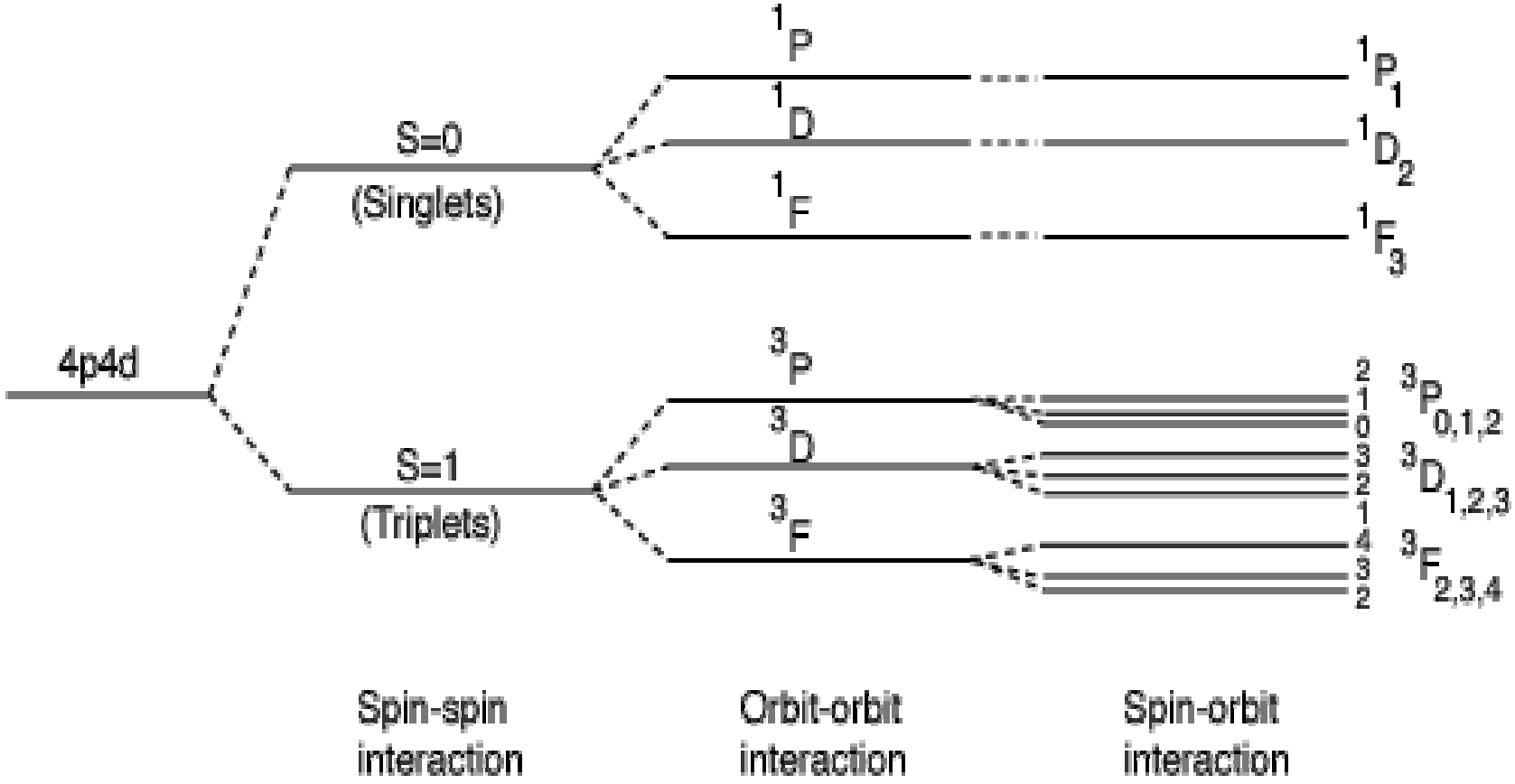
What is meant by *electronic structure*?



Atomic energy levels



What we calculate ?

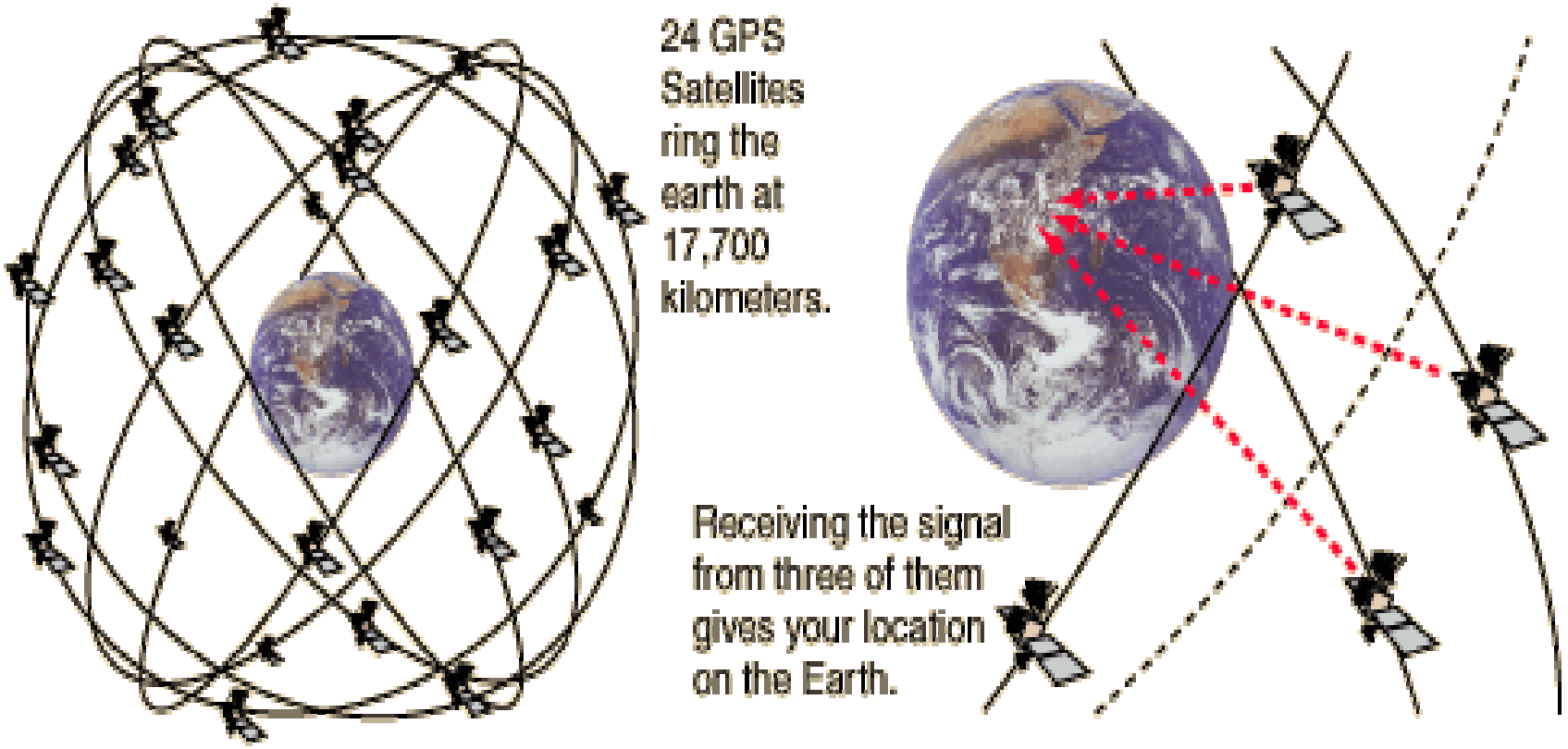
- Energies of atomic states
- Transition amplitudes
- Transition (lifetime) among different energy levels
- Hyperfine structure constants
- Parity violation in atoms
- Atomic electric dipole moment

Atomic clocks

1 second = 9,192, 631,770 cycles of the standard ^{133}Cs transition.

UTC (Universal Coordinated Time).

Atomic clocks are integral parts of the Global Positioning System (GPS) since extreme accuracy in timing is necessary



Ref :http://tycho.usno.navy.mil/cesium.html

Relativistic atomic Many-body theory

Information wanted

- Needs accurate numerical wavefunctions
- Appropriate numerical methods
- Corresponding algorithm

Different theories

- MCDF
- MBPT
- CI
- Green's Function
- Coupled Cluster

To solve a set of non-linear equations – which is CPU as well as memory intensive

1998 : Nobel Prize in Chemistry : Walter Kohn & John Pople
(*For Work on electronic structure and computational methods)*

EOM : QM treatment

$$H\Psi = E\Psi$$

In Coupled Cluster (CC) theory

$$\Psi = \exp(T)(1+S)\Phi$$

In CC the EOM takes the matrix form

$$A(T)\times T = B$$
$$A'(S)\times S = B'$$

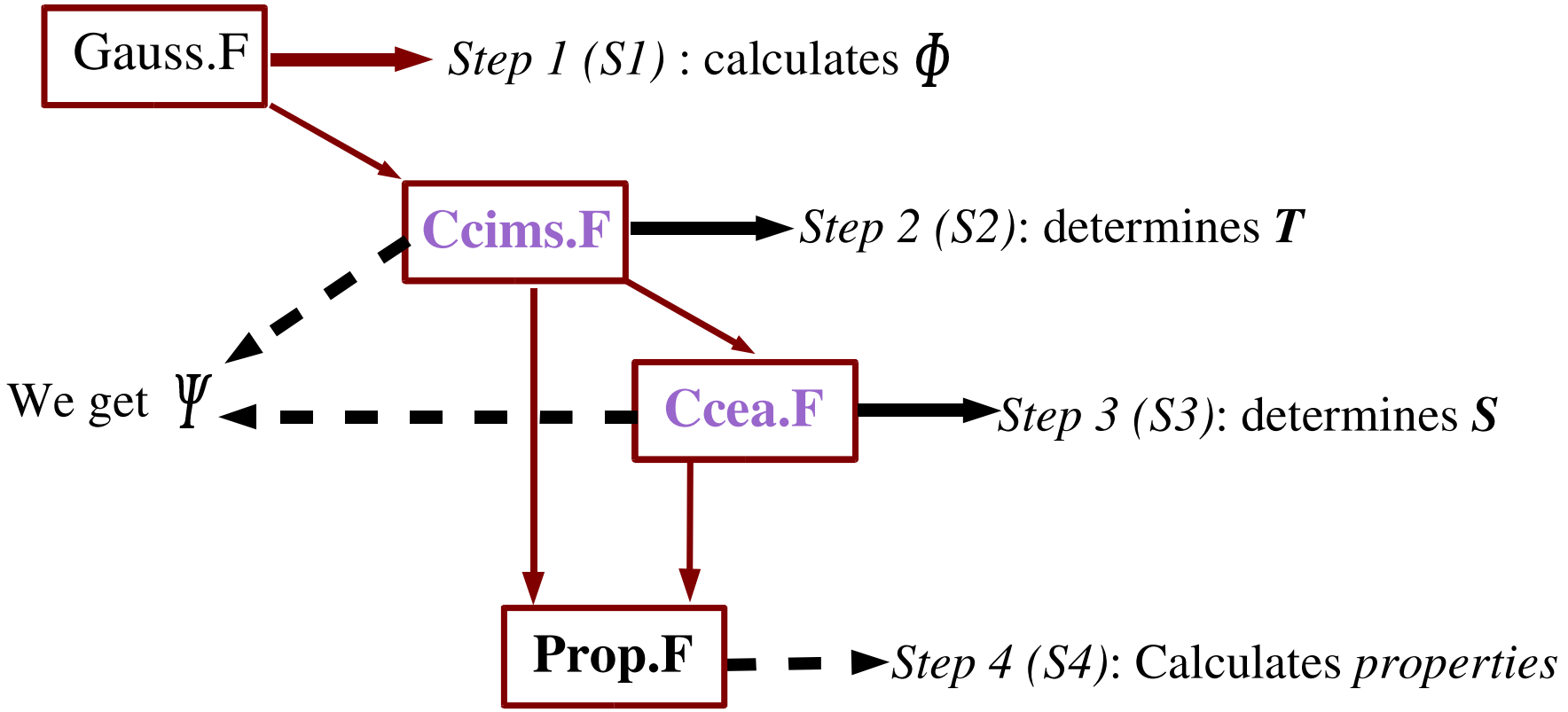
Explicit form

$$\begin{Bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \dots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{Bmatrix} \times \begin{Bmatrix} t_1 \\ t_2 \\ \vdots \\ t_n \end{Bmatrix} = \begin{Bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{Bmatrix}$$

- Any direct method to solve ? No way
- We use the **Jacobi algorithm** to solve it iteratively

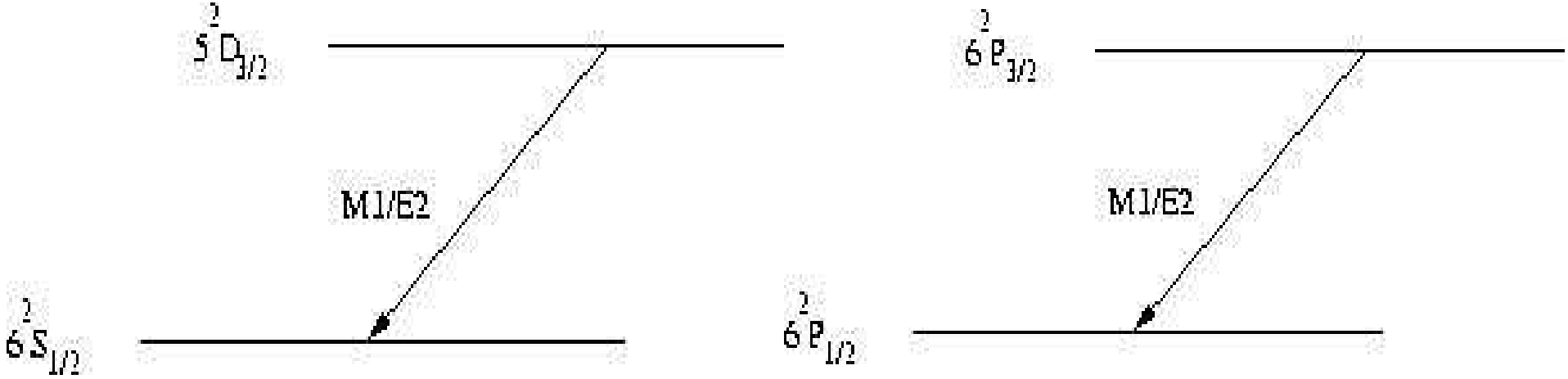
How we calculate ?

In several steps using a series of ***Fortran 77*** codes which depend on the earlier codes



Calculation of any atomic properties involves the exact wavefunction Ψ

Lifetime of excited states of atoms



Excited states of Ba^+ and Pb^+ ions

Transition probabilities for the decay of excited states are defined as

$$A_{fi}^{M1} = \frac{\left(2.6973 \times 10^{13}\right)}{\left[J_i\right]} \left(\Delta E\right)^3 S_{fi}^{M1}$$

$$A_{fi}^{E2} = \frac{\left(1.1199 \times 10^{18}\right)}{\left[J_i\right]} \left(\Delta E\right)^5 S_{fi}^{E2}$$

Lifetime (in *s*) is defined as

$$\tau = \frac{1}{A} = \frac{1}{\left(A^{M1} + A^{E2}\right)}$$

Some results

Lifetime (in *s*) of the excited states of Ba^+ and Pb^+ using Unitary Coupled Cluster (UCCSD(T)) theory

Ion	States	UCCSD(T)	Others (semi-empirical)	Experiment
Ba^+	$5^2D_{3/2}$	81.01	81.5 [1] 83.7 [2]	79 ± 4.6
Pb^+	$6^2P_{3/2}$	0.0413 0.0425 [3]		0.0412 ± 0.0007

[1] Dzuba *et al*, *Phys. Rev. A*, **63**, 062101 (2001).

[2] Guet *et al*, *Phys. Rev. A*, **44**, 1531 (1991).

[3] Our Group, CCSD(T), *J. Phys. B*, **37**, 3409 (2004).

Bottlenecks of the calculation – *CPU*

- *S2* and *S3* are hugely CPU and memory intensive
  - More than 2/3 time is spent on *S2* & *S3*

CPU mapping

Atom		PIV @2.4 GHz	SUN @450 MHz	Param Padma
Li (3)	*S2*	5m35.003s	16m37.67s	6m43.466s
	S3	7m12.31s	17m29.81s	8m35.386s
Cs (55)	*S2*	~14 hrs (Xeon)	~96 hrs	~9 hrs

Bottlenecks of the calculation – *memory*

Memory requirements mapping

PIV @2.4 GHz	SUN @450 MHz	Param Padma
	Memory available	
512 MB	4 GB	0.5 TB

Memory required (MB)		*S2*	*S3*
	Li (3)	300	350
	Rb(37)	500	700
	Cs (55)	1600	1900
	Pb (82)	3700	5500

Bottlenecks of the calculation – I/O

Dependent of the quality of HDD and system BUS

I/O mapping

PIV @2.4 GHz	SUN @450 MHz	Param Padma
7500 RPM (*IDE*) 100 MBps	10K RPM (*Ultra-SCSI*) 200 MBps	*Ultra-SCSI* ~1GBps

What kind of parallelisation ?

Mostly we do *SIMD* parallel programming

- Extensive use of MPI in different subroutines
  - Grouping of datas, use buffering
- Along with MPI, implementation of I/O (to make life simple for future)

Scaling of the MPI codes (CPU timings)

Atom	Xeon	SUN	Param Padma
Mg (12) *S2*	S :69m6.96s	S : ~203m	P1 :~25m, P6 :~6m
S3	S :78m6.48s		
Cs (55) *S2*	P3 :~500m	P3 :~900m	P3 : ~270m

Have a plan to do *MIMD* kind of task parallelism also - Seek help from you

Recent Publications

- *Ab initio* determination of lifetime of $6p_{3/2}$ state of Pb^+

  J. Phys. B, 2004

- Relativistic coupled-cluster calculation of core ionization potentials using the normal and semi-normal ordered antastz

  J. Phys. B, 2004

- Strong correlation effects in hyperfine interaction in Pb^+

  Submitted to *Phys. Rev. Lett., 2004*

- Comparative studies of magnetic dipole and electric quadrupole hyperfine constants for the ground and low lying excited states of $^{25}Mg^+$

  Euro. Phys. J. D, 2004

- Relativistic unitary coupled cluster theory and applications

  Submitted to *Phys. Rev.Lett., 2004*

Collaborations

Dr. Debasish Mukherjee and his group

IACS, Kolkata

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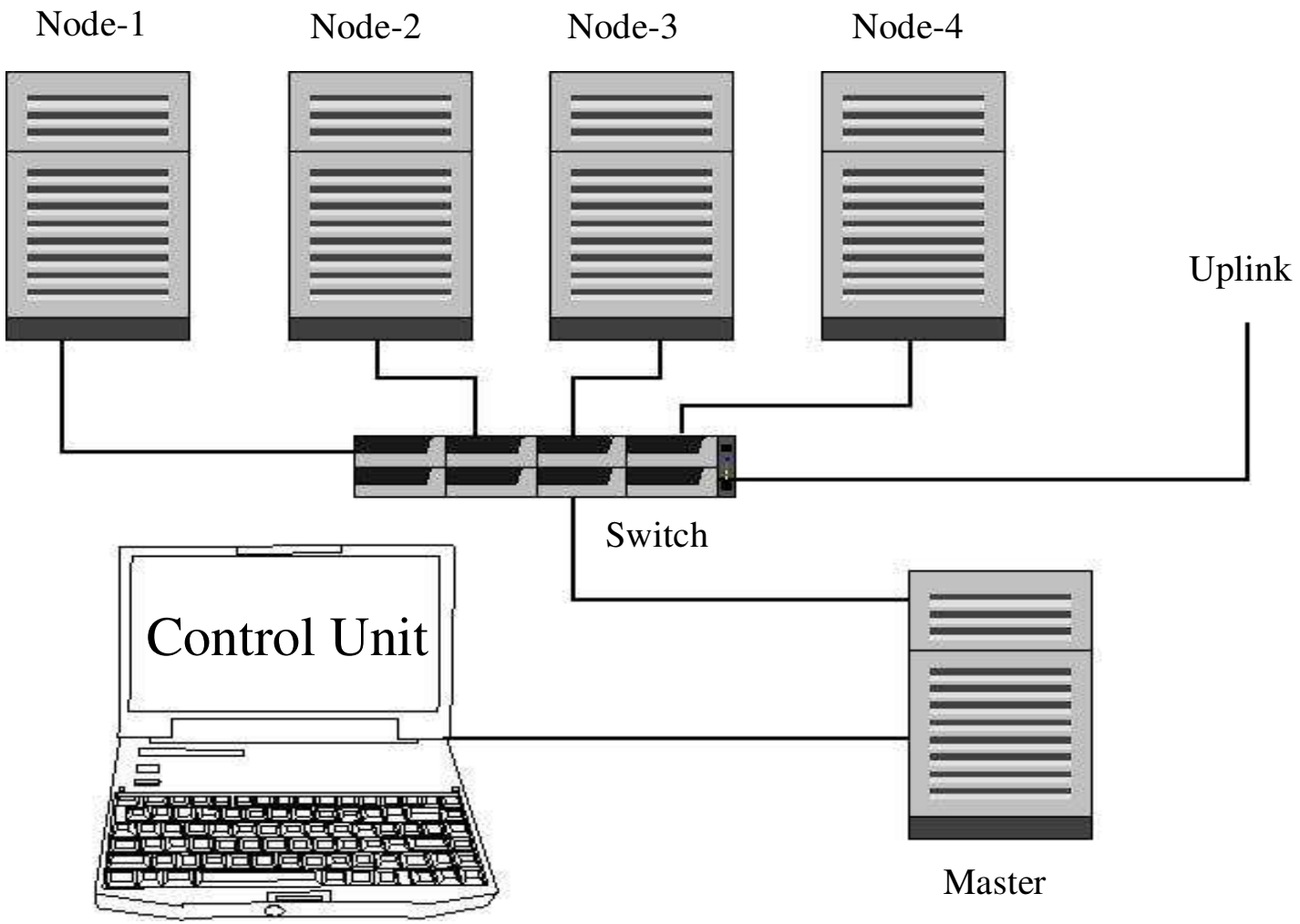
- Param Padma support team, CDAC, Bangalore

ATOMOS – Our cluster at NAPP



Our cluster ATOMOS @ NAPP

Compute Nodes

- Configuration : 5 Nos of 2 way SMP nodes
- Processors : Intel Xeon 2.66 Ghz
- File system : NFS
- Agreegate memory : 12 GB
- Operating system : RedHat Linux 9
  - Kernel : 2.4.20-8smp

Networks

Gigabit networks – (Netgear)

Software

- MPI-CH, MPI-LAM
- GNU compilers and Intel® compilers

Parallel computing – how is it ?