

An overview of the R-matrix electron-impact scattering package at NERSC

Workshop on Leadership-class Machines, Petascale Applications and Performance Strategies

July 27-30, Granlibakken Resort

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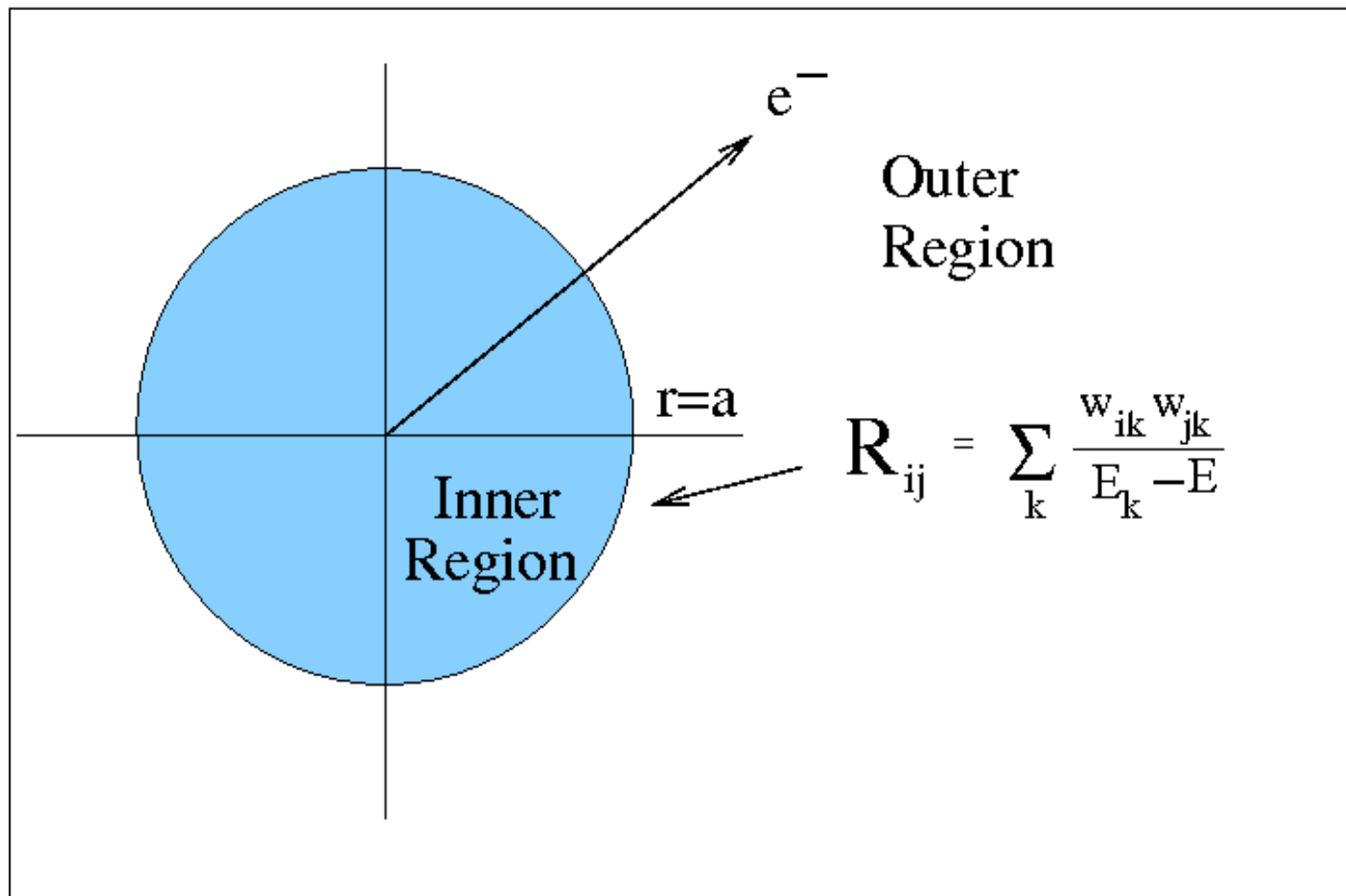
Auburn University

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: M S Pindzola

Acknowledgments : Dept of Energy
: NERSC

Structure of Talk

1. What is the R-matrix method ?
2. What is the underlying computational formalism and structure of the code base ?
3. Scaling up from 1000 -> 10000 processors on franklin.
4. Current bottlenecks/possible future directions



Computational Method

1. The formation of many real symmetric matrices (Hamiltonians), typically 60-100, requiring anywhere from 10-500 Gb of storage
2. The diagonalisation of each matrix, from which EVERY eigenvalue and EVERY eigenvector is required.

We achieve this through the `ScaLapack` package and in particular routines : `pdsyevx` and `pdsyevd`. Preference is given to the latter as it ensures orthogonality between all eigenvectors.

Matrices vary in size from $2K * 2K$ to $100K * 100 K$, depending on the complexity of the atomic target

LS coupling R-matrix (exchange) flowchart

INPUT

das/dauto

AUTOSTRUCTURE

OUTPUT

radial

dstg1

pstg1r

STG1.DAT
RKXXX.DAT

dstg2

pstg2r

STG2HXXX.DAT
sizeH.dat

dstg3

pstg3r

H.DAT

Outer Region

dstgf

pstgfg

OMEGA

FORMATION

DIAGONALISATION

PHYSICAL RESULT

pstgf is well tuned ... DGEMM and loop-unrolling, make future impact on code optimisation difficult!

FRANKLIN (2500 procs) during the dual core period

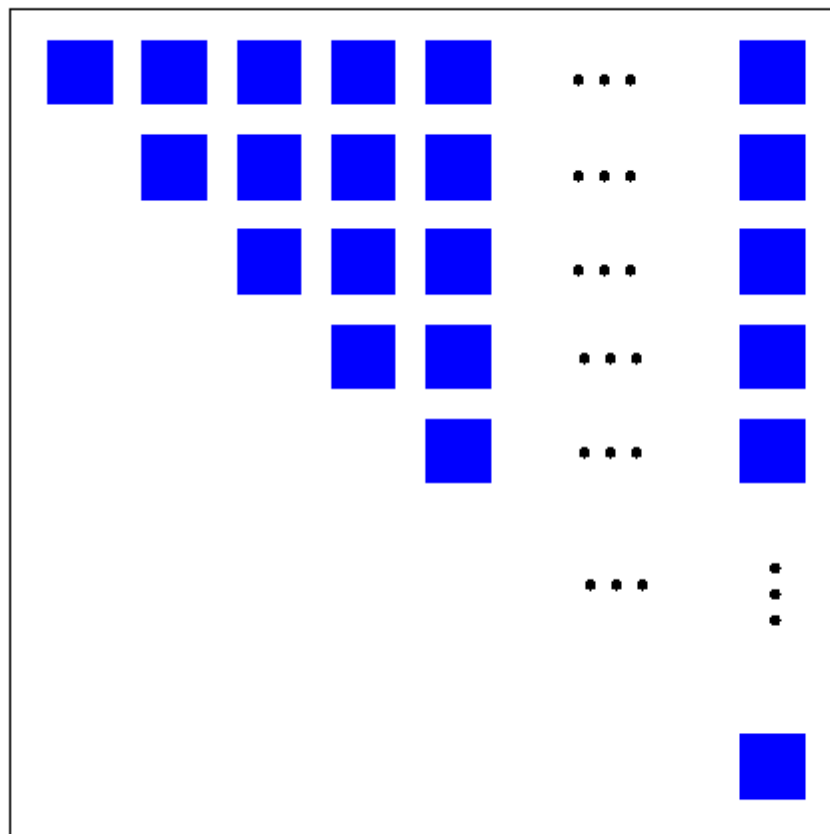
```
=====  
Totals for program  
-----  
Time%                100.0%  
Time                 7109.115661  
Imb.Time             21.832049  
Imb.Time%            0.3%  
Calls                404  
PAPI_TOT_INS         3045.675M/sec 20301132566037 instr  
PAPI_L1_DCA          1924.964M/sec 12830963966484 refs  
PAPI_FP_OPS          3107.882M/sec 20715780954715 ops  
DATA_CACHE_MISSES    49.228M/sec 328134470394 misses  
Cycles               6665.561 secs 17330459478592 cycles  
User time (approx)   6665.561 secs 17330459478592 cycles  
Utilization rate     93.8%  
Instr per cycle      1.17 inst/cycle  
HW FP Ops / Cycles   1.20 ops/cycle  
HW FP Ops / User time 3107.882M/sec 20715780954715 ops 59.8%peak  
HW FP Ops / WCT      2913.974M/sec  
HW FP Ops / Inst     102.0%  
Computation intensity 1.61 ops/ref  
MIPS                 7614187.14M/sec  
MFLOPS               7769706.07M/sec  
Instructions per LD ST 1.58 inst/ref  
LD & ST per D1 miss 39.10 refs/miss  
D1 cache hit ratio   97.4%  
LD ST per Instructions 63.2%  
=====
```

However plenty of progress to be made on the **formation** and **diagonalisation**

The formation of the scattering Hamiltonian

The formation of the continuum-continuum part of the N+1 electron Hamiltonian is the most time consuming

← Number of channels →



Therefore, if there are
several thousand scattering
channels

=

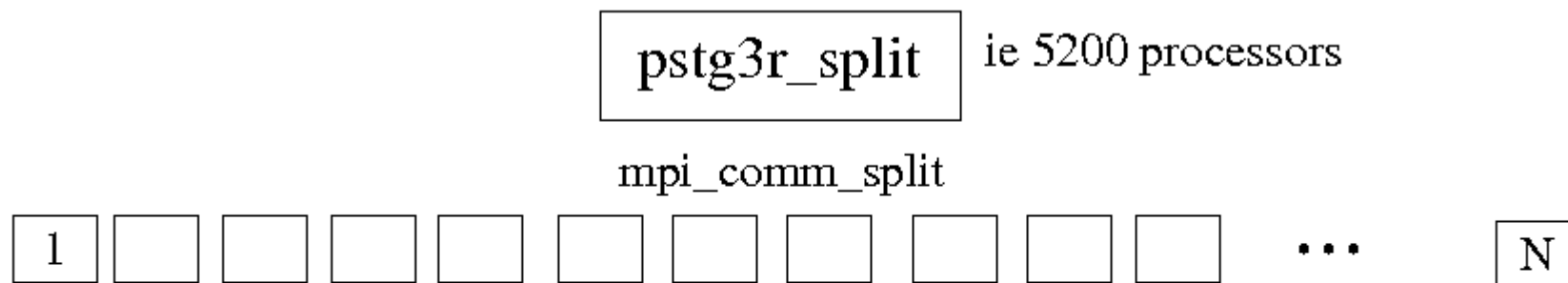
$$(NCHAN*(NCHAN+1))/2$$

matrix blocks !!!

i.e. several million

not very subtle, but effective ... parallel concurrent diagonalisation

(with help from NERSC consultants : Woo-Sun Yang ,Katie Antypas)



Each small box represents a partial wave

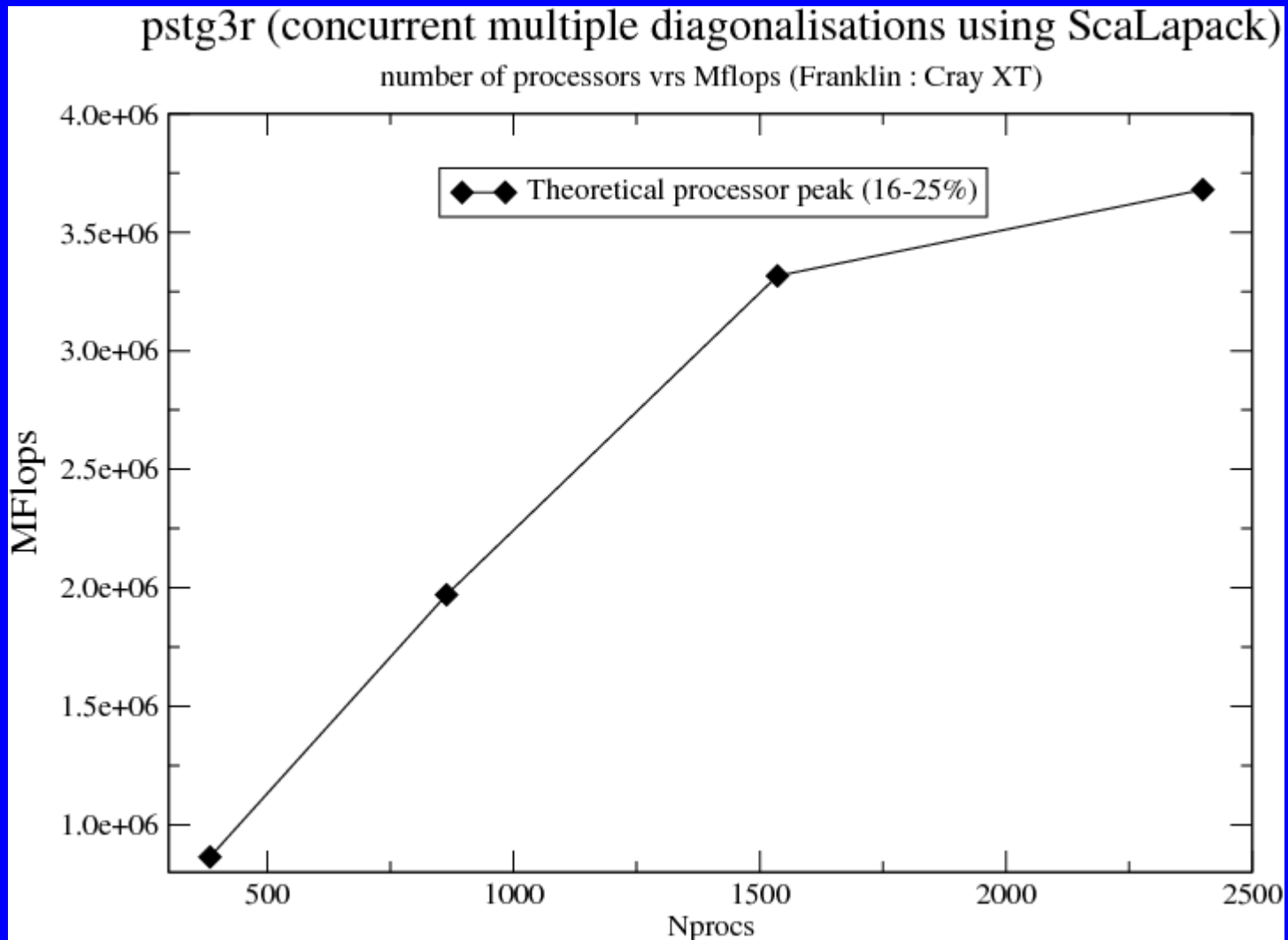
Each subgroup reads a single Hamiltonian and diagonalises it in parallel, concurrently with every other.

Almost endlessly scalable

Reduces all future R-matrix close-coupling calculations to the time required for a single partial wave.

Present situation when 'scaling up' on franklin

96 matrices , each 10721*10721 in dimension



sample profiling for the same case ...

```
pstg3r.profile.txt - /home/connor/latex/workshop/
File Edit Search Preferences Shell Macro Windows Help
=====
Totals for program
-----
Time%                100.0%
Time                179.868711 secs
Inb.Time            0.485217 secs
Inb.Time%           0.3%
Calls                2.6 /sec      405.0 calls
RETIRED_MMX_AND_FP_INSTRUCTIONS:
  PACKED_SSE_AND_SSE2 1722.618M/sec 272399534900 instr
  PAPI_FML_INS        1076.992M/sec 170305883797 ops
  PAPI_FAD_INS        1081.897M/sec 171081650827 ops
  PAPI_FDV_INS         2.185M/sec  345548107 ops
  User time (approx)  158.131 secs 363701551563 cycles 87.9%Time
  Average Time per Call 0.444120 sec
  CrayPat Overhead : Time 0.0%
  HW FP Ops / Cycles 0.94 ops/cycle
  HW FP Ops / User time 2158.889M/sec 341387534625 ops 23.5%peak(DP)
  HW FP Ops / WCT 1897.982M/sec
  FP Multiply / FP Ops 49.9%
  FP Add / FP Ops 50.1%
  MFLOPS (aggregate) 3316053.72M/sec
=====
```

In a nutshell ,one of the biggest remaining challenges to continued scaling of the problem is:

the construction of the Hamiltonian,

then distributing the pertinent information to

a particular processor,
in a particular ScaLapack context,
before diagonalisation.