

Overview of Parallel Maths Libraries

Gavin Pringle

gavin@epcc.ed.ac.uk

Overview

- Why Libraries?
- Linear Algebra
 - Matrix types
 - Serial Libraries
 - BLAS and LAPACK
 - Parallel Libraries
 - ScaLAPACK
- PDEs
 - PETSc
- FFTs
 - FFTW
 - Parallel FFTs

Libraries

Why Use Libraries?

- Easier
 - save effort and time, no duplicated code
- Avoid bugs
 - libraries are (hopefully) well tested
- Performance
 - usually contain efficient implementations,
 - perhaps optimised for a given system (vendor-specific architectures), or
 - auto-tuning

What is a Library?

- Collection of pre-implemented routines available in some sort of package
 - static archive, shared library, Framework, DLL, etc.
- Defined (and hopefully documented) API
- Often provided with operating system (e.g. Scientific Linux), available via package managers, or binary/source downloads
- Can be combined with your code by linking (and perhaps #including header files)

Basic Linear Algebra Matrices

Matrix types

- Matrices generally classified as either *sparse* or *dense*
 - We will deal with sparse matrices later
- Rectangular matrices
 - correspond to different number of equations from unknowns
 - system can be either under- or over-determined
- Matrices may have symmetry about the diagonal:
 - Symmetric (real matrices): $a_{ij} = a_{ji} \rightarrow A^T = A$
 - Hermitian (complex matrices): $a_{ij}^* = a_{ji} \rightarrow A^{T*} = A^\dagger = A$

$$\begin{array}{ccc} \mathbb{R} & 1 & 2 \\ \mathbb{C} & 2 & 3 \\ \mathbb{R} & 2 & 3 \end{array}$$

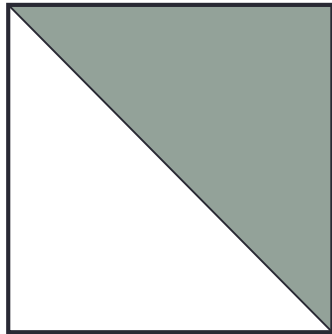
Symmetric

$$\begin{array}{ccc} \mathbb{R} & 1 & 2 + i \\ \mathbb{C} & 2 - i & 3 \\ \mathbb{R} & 2 - i & 3 \end{array}$$

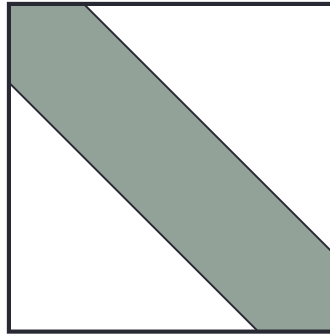
Hermitian

Matrix structures

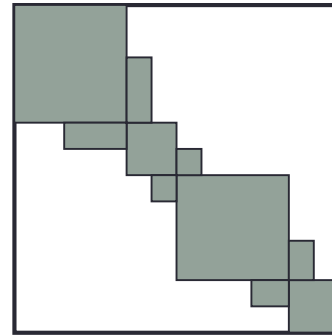
- Many matrices have a regular structure



Upper
triangular



Band
diagonal



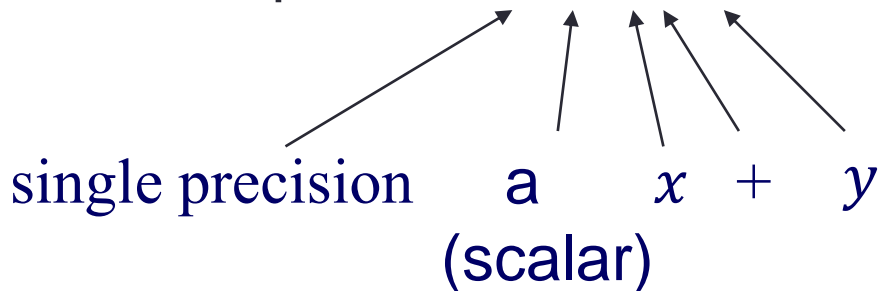
Block
diagonal

Serial Linear Algebra Libraries

BLAS

- Basic Linear Algebra Subprograms
 - Level 1: vector-vector operations (e.g. $x \cdot y$)
 - Level 2: matrix-vector operations (e.g. Ax)
 - Level 3: matrix-matrix operations (e.g. AB)
(x, y vectors, A, B matrices)

- Example: SAXPY routine



y is replaced “in-place” with $a x + y$

SAXPY

- In Fortran

```
call SAXPY(n,a,x,incx,y,incy)
```

```
...
```

```
ix = 1; iy = 1
```

```
do i = 1, n
```

```
    y(iy) = y(iy) + a * x(ix)
```

```
    ix = ix + incx; iy = iy + incy
```

```
end do
```

LAPACK

- LAPACK is built on top of BLAS libraries
 - Most of the computation is done with the BLAS libraries
- Original goal of LAPACK was to run efficiently on shared memory and multi-layered systems
 - Spend less time moving data around!
- LAPACK attempts to use BLAS 3 instead of BLAS 1
 - matrix-matrix operations more efficient than vector-vector
- Illustrates trend to layered numerical libraries
 - allows for portable performance libraries
 - efficient implementation of BLAS 3 leads immediately to efficient implementation of LAPACK
 - porting LAPACK becomes a straightforward exercise

BLAS/LAPACK naming conventions

- Routines generally have a name of up to 6 letters, e.g. DGESV,
- Initial letter
 - S: Real C: Complex
 - D: Double Precision Z: Double Complex or COMPLEX*16
- For level 2 and 3 routines, 2nd and 3rd letter refers to matrix type
 - GE: matrices are general rectangular
 - i.e. could be unsymmetric, not necessarily square
 - HE: (complex) Hermitian
 - SY: symmetric
 - TR: triangular
 - BD: bidiagonal
 - etc.
 - ~30 in total
- E.g. SGESV: Single precision, general matrix solver (solves $A x = b$)

Sparse matrices

- Direct methods easiest for structured matrices
 - E.g. tridiagonal, pentadiagonal, block-diagonal
 - support in LAPACK for some well-structured sparse cases
- General sparse matrices
 - difficult to code efficiently due to “fill-in”
 - LU factors will have non-zero entries even where A was zero
 - some specialist libraries,
 - e.g. HSL (formerly the **Harwell Sparse Matrix Library**)
- In general, iterative methods are used

Parallel Dense Linear Algebra Library

Parallel dense linear algebra libraries

- ScaLAPACK is basically a parallel version of LAPACK with a few extra routines
 - E.g. matrix transposition
 - Some LAPACK routines have been improved to help with scalability
- Large **sparse** matrices: instead use **ARPACK** or parallel equivalent (**P_ARPACK**)

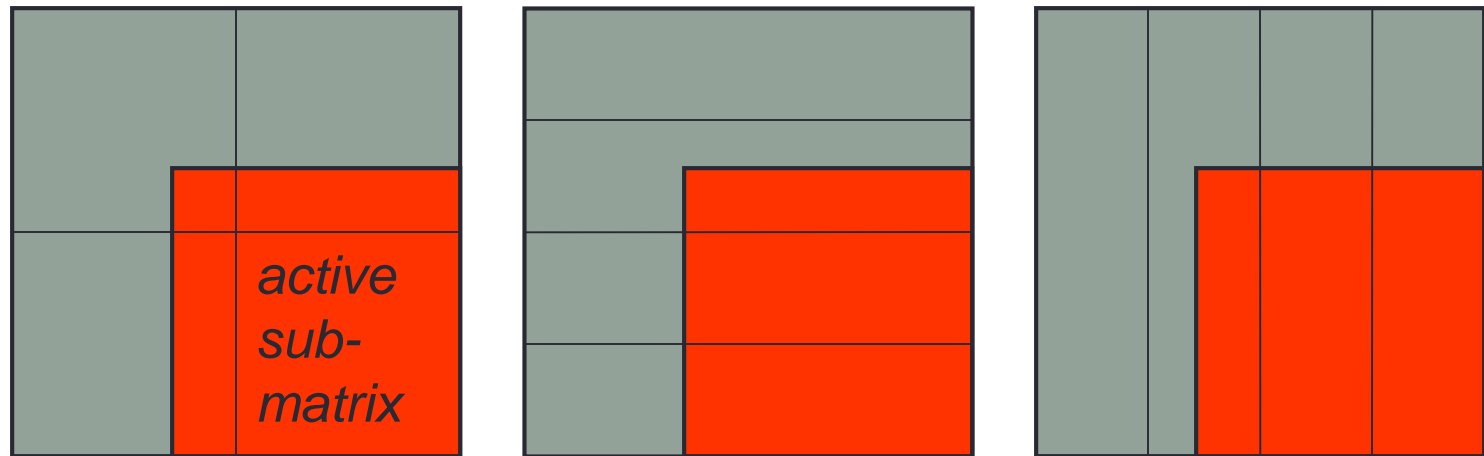
Dense Linear Algebra in parallel

- Consider LU factorisation
 - equivalently Gaussian Elimination
- Main operations were
 - `saxpy` – for subtracting one row from another
 - `dgemm` – matrix-matrix multiplication – scaling
- Algorithm works on progressively smaller sub-matrix
 - More zeros on each row as you move down the matrix

$$\begin{bmatrix} a'_{11} & a'_{12} & a'_{13} & a'_{14} \\ 0 & a'_{22} & a'_{23} & a'_{24} \\ 0 & a'_{32} & a'_{33} & a'_{34} \\ 0 & a'_{42} & a'_{43} & a'_{44} \end{bmatrix} \rightarrow \begin{bmatrix} a'_{11} & a'_{12} & a'_{13} & a'_{14} \\ 0 & a'_{22} & a'_{23} & a'_{24} \\ 0 & 0 & a'_{33} & a'_{34} \\ 0 & 0 & a'_{43} & a'_{44} \end{bmatrix} \rightarrow \dots$$

Parallelisation

- Clear opportunities for parallelism
 - multiple independent **saxpy** or **SGEMM** operations
 - major problem is load balance, on four processors

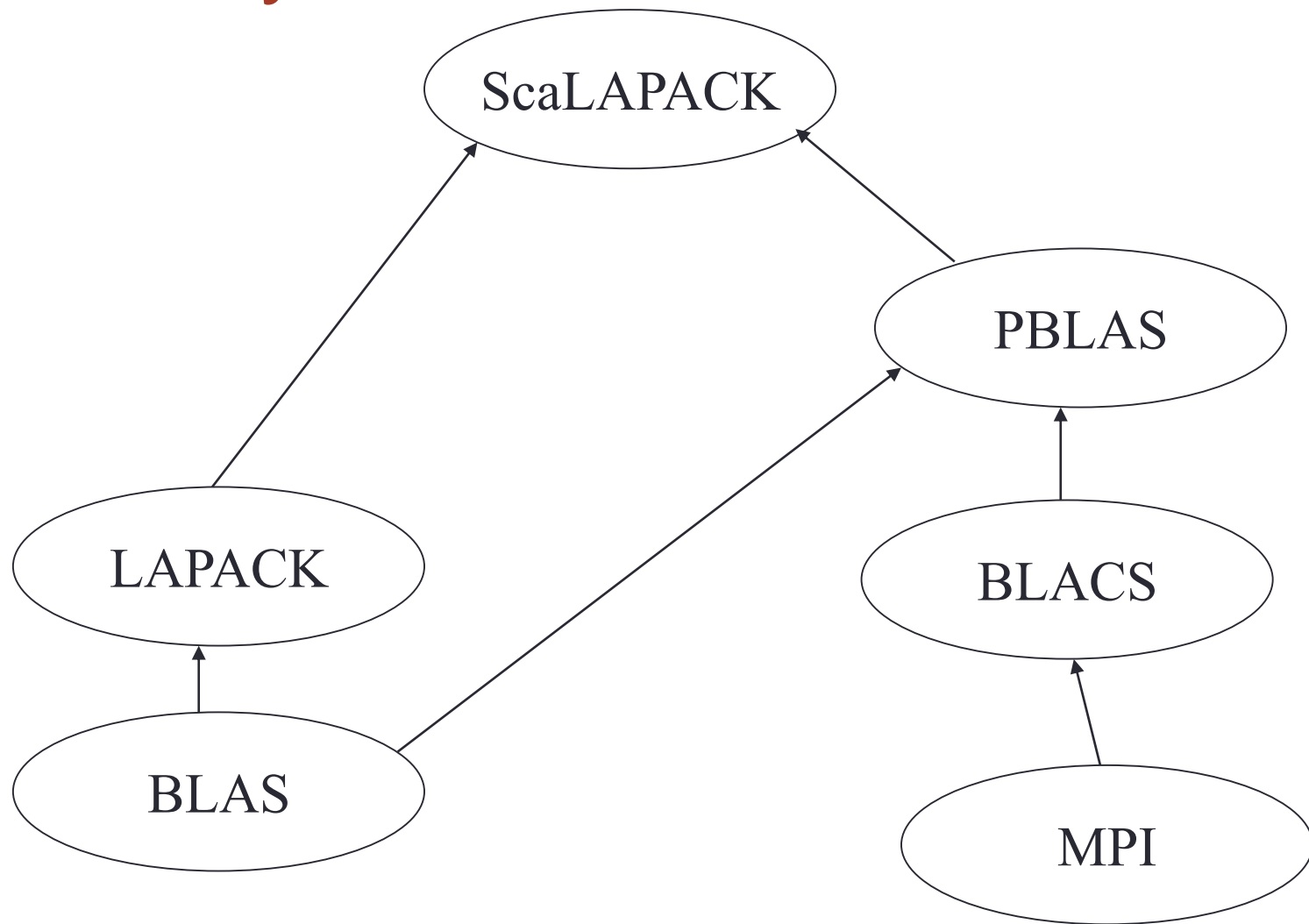


- No simple block distribution is appropriate
 - But clear we must use block-cyclic in at least one dimension

ScaLAPACK introduction

- ScaLAPACK allows us to run LAPACK-like routines *in parallel*
- Routines written to resemble equivalent LAPACK routines
 - e.g. dgesv → pdgesv
- Assumes matrices are laid out in 2D block-cyclic form
 - In contrast to sparse matrices - usually 1D decomposition
- Built on top of
 - LAPACK (Linear algebra library)
 - PBLAS (distributed memory version of Level 1, 2 and 3 BLAS)
 - BLACS (Basic Linear Algebra Communication Subprograms)
 - MPI
- As with LAPACK, written in Fortran 77 but interfaces to Fortran 90/C/C++

Hierarchy



ScaLAPACK

- ScaLAPACK follows similar format to MPI
 - BLACS “context” being the equivalent of an MPI communicator
 - Need several set-up and finalise routines
- Matrices/vectors completely distributed over processors and described using an *array descriptor*
- Set up a 2D processor grid
 - Routines provided to determine processor position in grid and local matrix size
- Data distributed in a “block cyclic” fashion with block size (referred to as “blocking factor”)
 - ScaLAPACK describes this as “complicated but efficient”

2D Block cyclic

- Situation can be simple – e.g. 8×8 matrix with 2×2 processor grid...

P ₀	P ₀	P ₀	P ₀	P ₁	P ₁	P ₁	P ₁
P ₀	P ₀	P ₀	P ₀	P ₁	P ₁	P ₁	P ₁
P ₀	P ₀	P ₀	P ₀	P ₁	P ₁	P ₁	P ₁
P ₀	P ₀	P ₀	P ₀	P ₁	P ₁	P ₁	P ₁
P ₂	P ₂	P ₂	P ₂	P ₃	P ₃	P ₃	P ₃
P ₂	P ₂	P ₂	P ₂	P ₃	P ₃	P ₃	P ₃
P ₂	P ₂	P ₂	P ₂	P ₃	P ₃	P ₃	P ₃
P ₂	P ₂	P ₂	P ₂	P ₃	P ₃	P ₃	P ₃

- ...or by making processor blocks smaller can be more complicated...

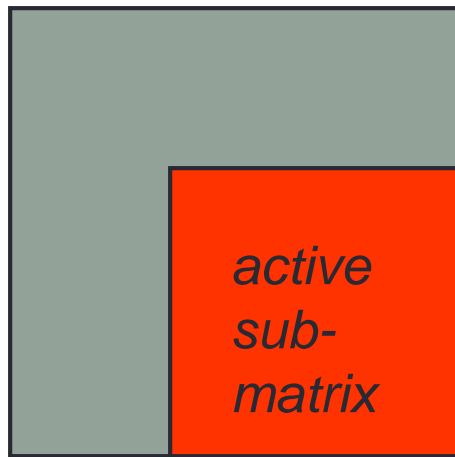
P ₀	P ₀	P ₁	P ₁	P ₀	P ₀	P ₁	P ₁
P ₀	P ₀	P ₁	P ₁	P ₀	P ₀	P ₁	P ₁
P ₂	P ₂	P ₃	P ₃	P ₂	P ₂	P ₃	P ₃
P ₂	P ₂	P ₃	P ₃	P ₂	P ₂	P ₃	P ₃
P ₀	P ₀	P ₁	P ₁	P ₀	P ₀	P ₁	P ₁
P ₀	P ₀	P ₁	P ₁	P ₀	P ₀	P ₁	P ₁
P ₂	P ₂	P ₃	P ₃	P ₂	P ₂	P ₃	P ₃
P ₂	P ₂	P ₃	P ₃	P ₂	P ₂	P ₃	P ₃

2D block cyclic distribution - example

- Global matrix size: 9×9
- Block size: 2×2
- No. processors: 6
- Processor grid: 2×3
- Local matrix sizes
 - P_0 : $5 \times 4 = 20$
 - P_1 : $5 \times 3 = 15$
 - P_2 : $5 \times 2 = 10$
 - P_3 : $4 \times 4 = 16$
 - P_4 : $4 \times 3 = 12$
 - P_5 : $4 \times 2 = 8$
- Routines exist to calculate local sizes

P_0	P_0	P_1	P_1	P_2	P_2	P_0	P_0	P_1
P_0	P_0	P_1	P_1	P_2	P_2	P_0	P_0	P_1
P_3	P_3	P_4	P_4	P_5	P_5	P_3	P_3	P_4
P_3	P_3	P_4	P_4	P_5	P_5	P_3	P_3	P_4
P_0	P_0	P_1	P_1	P_2	P_2	P_0	P_0	P_1
P_0	P_0	P_1	P_1	P_2	P_2	P_0	P_0	P_1
P_3	P_3	P_4	P_4	P_5	P_5	P_3	P_3	P_4
P_3	P_3	P_4	P_4	P_5	P_5	P_3	P_3	P_4
P_0	P_0	P_1	P_1	P_2	P_2	P_0	P_0	P_1

2D block cyclic applied to LU factorisation



P ₀	P ₀	P ₁	P ₁	P ₂	P ₂	P ₀	P ₀	P ₁
P ₀	P ₀	P ₁	P ₁	P ₂	P ₂	P ₀	P ₀	P ₁
P ₃	P ₃	P ₄	P ₄	P ₅	P ₅	P ₃	P ₃	P ₄
P ₃	P ₃	P ₄	P ₄	P ₅	P ₅	P ₃	P ₃	P ₄
P ₀	P ₀	P ₁	P ₁	P ₂	P ₂	P ₀	P ₀	P ₁
P ₀	P ₀	P ₁	P ₁	P ₂	P ₂	P ₀	P ₀	P ₁
P ₃	P ₃	P ₄	P ₄	P ₅	P ₅	P ₃	P ₃	P ₄
P ₃	P ₃	P ₄	P ₄	P ₅	P ₅	P ₃	P ₃	P ₄
P ₀	P ₀	P ₁	P ₁	P ₂	P ₂	P ₀	P ₀	P ₁

- This decomposition allows a reasonable load balance

ScaLAPACK: Example solving $Ax=b$

```
...
n=64; nrhs=1; nprow=2; npcol=3; mb=nb=2;
...
CALL BLACS_GET(-1,0,ctxt)
CALL BLACS_GRIDINIT(ctxt, 'Row-major', nprow, npcol)
CALL BLACS_GRIDINFO(ctxt, nprow, npcol, myrow, mycol)
...
num_rows_local = NUMROC(n, nb, myrow, 0, nprow)
num_cols_local = NUMROC(n, nb, mycol, 0, npcol)
...
Allocate(A(num_rows_local, num_cols_local), b(num_rows_local),
ipiv(num_rows_local+nb))
...
IF(MYROW.EQ.-1) Skip computation!
...
CALL DESCINIT(desca, n, n,      mb, nb,      rsrc, csrc ,ctx, llda ,info)
CALL DESCINIT(descb, n, nrhs, nb ,nbrhs, rsrc, csrc, ctx, lldb, info)
...
call PDGETRF(n, n, A, 1, 1, desca, ipiv, info)
call PDGETRS('N', n, 1, A, 1, 1, desca, ipiv, b, 1, 1, descb, info)
...
WRITE(*,*) ...Results.....
...
CALL BLACS_EXIT(0)
```

Brief Diversion

Calling Fortran Libraries from C

Calling Fortran libraries from C

- A number of issues
 - storage order of matrices
 - calling by reference / calling by value
 - character variables
 - subroutine names
- C arrays are transposed w.r.t. Fortran
 - could choose to store all matrices in transpose format
 - but may simply be able to specify **TRANS= 'T'** where appropriate
- Fortran *always* expects pass-by-reference
 - must assign C constants to variables, eg **one = 1;**
 - pass the pointer **&one** to the subroutine

System Dependent

Calling LAPACK from C

- Fortran

```
call SGETRS (TRANS, N, NRHS, A, LDA, IPIV, B, LDB, INFO)
```

- Easiest to write a wrapper for C, e.g:

```
int sgetrs(char trans, int n, int nrhs,  
float *a, int lda, int *ipiv, float *b, int ldb)  
{  
    int info;  
    sgetrs_(&trans, &n, &nrhs, a, &lda, ipiv, b, &ldb, &info);  
    return(info);  
}  
...  
info = sgetrs('t', n, 1, &(a[0][0]), NMAX, ipiv, x, NMAX);
```

C requires the following libs when linking:

```
-llapack -lblas -lpgftnrtl -lrt
```

Parallel Partial Differential Equation solvers

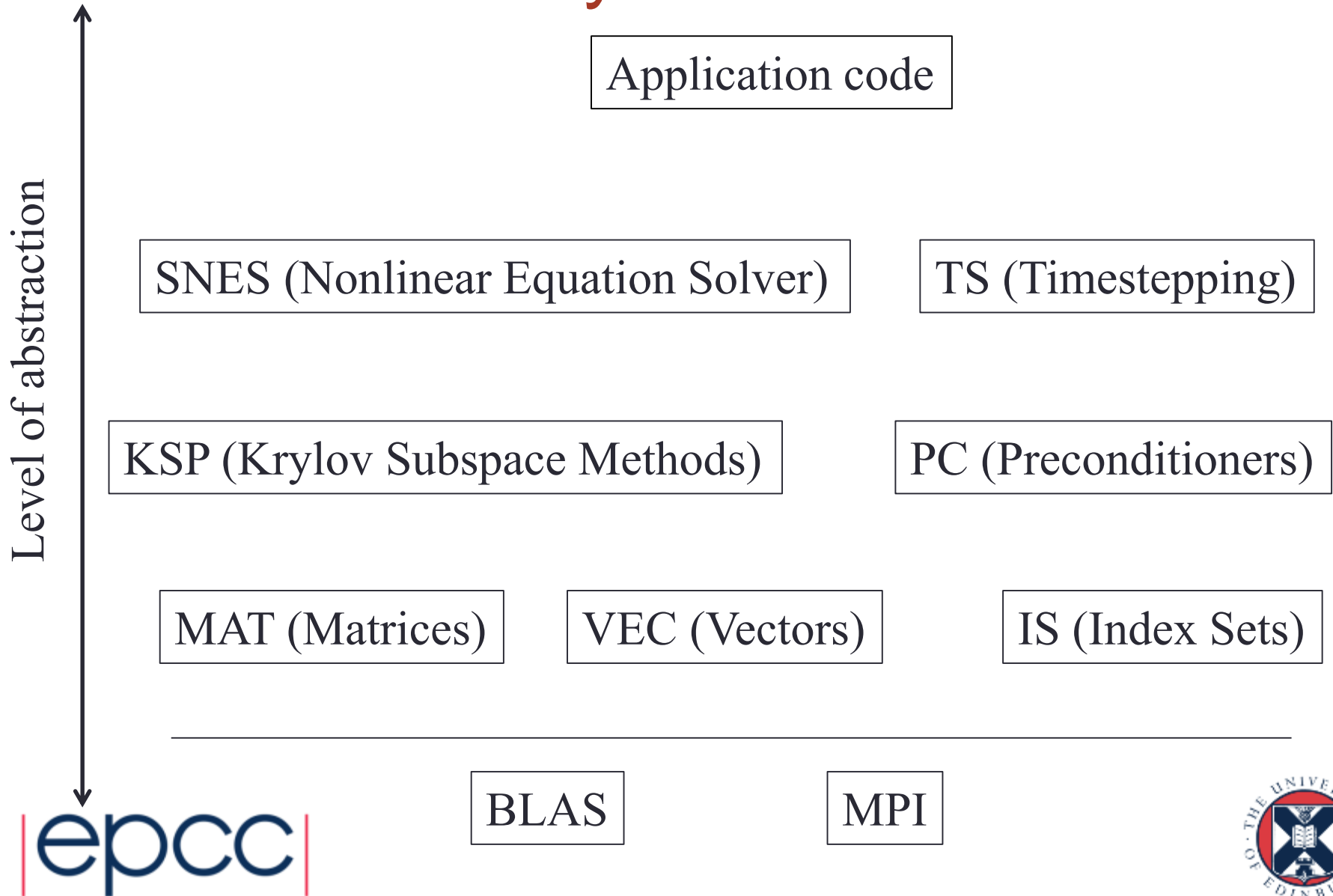
PETSc

- The Portable, Extensible Toolkit for Scientific computing
 - <http://www.mcs.anl.gov/petsc/petsc-as/>
 - Pronounced PET-see (the S is silent)
- Suite of data structures and routines for the parallel solution of Partial Differential Equations.
 - PDEs
- It supports MPI, and GPUs through
 - CUDA or OpenCL, as well as
 - hybrid MPI-GPU parallelism.
- Current PETSc version is 3.12

PETSc use in codes

- There are many, but notable examples
 - SLEPc
 - Scalable Library for Eigenvalue Problems
 - Fluidity
 - a finite element/volume fluids code
 - libMesh
 - adaptive finite element library
 - FEniCS and Firedrake
 - sophisticated Python based finite element simulation package
 - ...

PETSc Hierarchy



Design characteristics

- Distributed memory programming only
 - No shared/global variables
- Object-oriented
- Callable from C, C++, Fortran, Python
- Same code runs in serial or parallel
- Either real or complex scalar datatype
 - library build option,
 - your code doesn't look different

Example

```
#include <petsc.h>

int main(int argc, char **argv)
{
    Vec x;
    PetscInt n = 100;
    PetscScalar y;
    PetscInitialize(&argc, &argv,
                   PETSC_NULL,
                   PETSC_NULL);
    VecCreate(PETSC_COMM_WORLD, &x);
    VecSetSizes(x, PETSC_DECIDE, n);
    VecSetFromOptions(x);
    VecSetRandom(x, PETSC_NULL);
    VecDot(x, x, &y);

    PetscPrintf(PETSC_COMM_WORLD,
               "Dot product is %g\n", y);
    VecDestroy(&x);
    PetscFinalize();
    return 0;
}
```

```
program main
#include "finclude/petscdef.h"
use petsc
implicit none
Vec :: x
PetscInt :: n = 100
PetscScalar :: y
integer :: ierr
character(len=12) :: tmp
call PetscInitialize(PETSC_NULL_CHARACTER, &
                    ierr)
call VecCreate(PETSC_COMM_WORLD, x, ierr)
call VecSetSizes(x, PETSC_DECIDE, n, ierr)
call VecSetFromOptions(x, ierr)
call VecSetRandom(x, PETSC_NULL_OBJECT, ierr)
call VecDot(x, x, y, ierr)

write(tmp, '(F10.5)')y
call PetscPrintf(PETSC_COMM_WORLD, &
                'Dot product is'//trim(tmp)//'\n', &
                ierr)
call VecDestroy(x, ierr)
call PetscFinalize(ierr)
end program main
```

Parallel Fast Fourier Transforms

Who would use Fourier Transforms?

- Physical Sciences

- Cosmology (P^3M N-body solvers)
- Fluid mechanics
- Computational Chemistry
- Quantum physics
- Signal and image processing
 - Antenna studies
 - Optics

Caveat: different disciplines use different notation, normalisation, and sign conventions

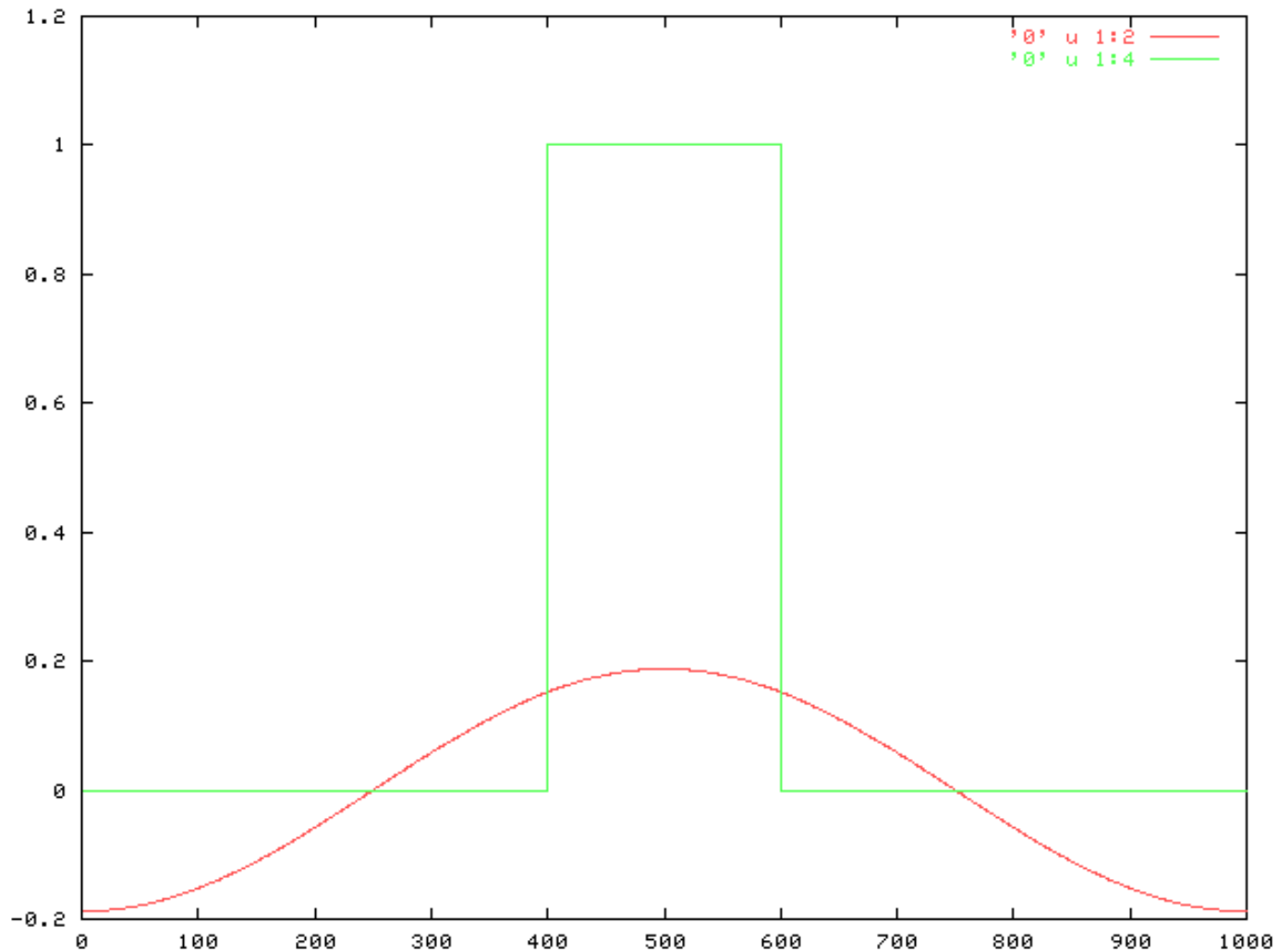
- Numerical analysis

- Linear systems analysis
- Boundary value problems
- Large integer multiplication (Prime finding)

- Statistics

- Random process modelling
- Probability theory

Example: The Top Hat Function



Mathematics of the Fourier Transform

- The Fourier Transform of a complex function $f(x)$

$$F(s) = \int_{-\infty}^{\infty} f(x)e^{-i2\pi xs} dx$$

- The inverse Fourier Transform

$$f(x) = \int_{-\infty}^{\infty} F(s)e^{i2\pi xs} ds$$

Discrete Fourier Transform

- The Discrete Fourier Transform of N complex points f_k is defined as

$$F_n = \sum_{k=0}^{N-1} f_k e^{2\pi i k n / N}$$

- The inverse Discrete Fourier Transform, which recovers the set of f_k values exactly from the F_n values is

$$f_k = \frac{1}{N} \sum_{n=0}^{N-1} F_n e^{-2\pi i k n / N}$$

Discrete Fourier Transform

- The DFT can be rewritten as

$$F_n = a_0 + \sum_{k=1}^{N-1} \left(a_k \cos \left(2\pi k \frac{n}{N} \right) + b_k i \sin \left(2\pi k \frac{n}{N} \right) \right)$$

- Thus, the DFT essentially returns real number values for a_k and b_k , stored in a complex array
 - a_k and b_k are functions of f_k
 - remaining trigonometric constants (twiddle factors) may be pre-computed for a given N

Fast Fourier Transform

- In 1965, J.W. Cooley and J.W. Tukey published a DFT algorithm which is of $\mathcal{O}(N \log N)$
 - Fast Fourier Transform (FFT)
- N must be a power of 2
 - FFTs in general are not limited to powers of 2, however, the order may resort to $\mathcal{O}(N^2)$
 - Essentially a divide-and-conquer algorithm
- In hindsight, faster than $\mathcal{O}(N^2)$ algorithms were previously, independently discovered
 - Gauss was probably first to use such an algorithm in 1805

FFT Libraries

- FFTs do not normalise
 - Each FFT/Inverse FFT pair scales by a factor of N
 - Usually left as an exercise for the programmer.
- DFTs are complex-to-complex transforms, however, most applications require real-to-complex transforms
 - Simple solution: set imaginary part of input data to be zero
 - This will be relatively slow
 - May be better to pack and unpack data
 - Place all the real data into all slots of the input, complex array (of length $N/2$) and then unpack the result on the other side ($\mathcal{O}(N)$)
 - Around twice as fast as the simple solution
 - Good details in Numerical Recipes book
 - Some libraries have real-to-complex wrappers
 - Similar approach allows us to do 2 independent real-to-complex transforms simultaneously

FFT Libraries

- Multidimensional FFTs
 - simply successive FFTs over each dimension
 - order immaterial: linearly independent operations
 - can place data into 1D array
 - strided FFTs
 - some libraries have multidimensional FFT wrappers
- Parallel FFTs
 - performing FFT on distributed data
 - 1D FFTs are cumbersome to parallelise
 - Suitable only for huge N
 - 2D, 3D, 4D, ..., parallel, array transpose operation
 - distributed data is collated on one processor before FFT
 - more in parallel libraries lecture later
 - some libraries have parallel FFT wrappers

FFTW

- Fastest Fourier Transform in the West
 - www.fftw.org
- The FFTW package was developed at MIT by Matteo Frigo and Steven G. Johnson
- Free under GNU General Public License
- Portable, self-optimising C code
 - Runs on a wide range of platforms
- Arbitrary sized FFTs of one or more dimensions
 - Fastest routines where N is composed of
 - powers of 2, 3, 5 and 7 and
 - multiples of 11 and 13, and
 - other sizes can be optimised for at configuration time

FFTW: FFTW2 vs FFTW3

- Previous version: “FFTW2”
 - Many legacy codes employ FFTW2
 - Simple(r) C interface, with wrappers for many other languages
 - Supports MPI
 - Rest of this lecture assumes “FFTW2”
- New version: “FFTW3”
 - Different interface to FFTW2 – to allow planner more freedom to optimise
 - Users must rewrite code
 - Supports MPI (now)
 - Somewhat faster than FFTW2 (~10% or more)

FFTW: Details

- Can perform FFTs on distributed data
 - MPI for distributed memory platforms
 - OpenMP or POSIX for SMPs
- If users rewrite their code to this FFT just once then the user is saved from
 - learning platform dependent, proprietary FFT routines
 - rewriting their code every time they port their code
 - No standard interface to FFTs
 - drastically rewriting their makefiles
 - location of FFTW libraries may vary
- FORTRAN wrappers for the majority of routines
- FFTs can not always be done “in-place”
 - The input and output arrays must be separate and distinct or temp arrays created

FFTW: Plans

- All FFT libraries pre-compute the *twiddle factors*
- FFTW ‘plans’ also generates the FFT code from *codelets*
 - Codelets compiled when FFTW configured
- Two forms of plans
 - Estimated
 - The best numerical routines are guessed, based on information gleaned from the configuration process.
 - Measured
 - Different numerical routines are actually run and timed with the fastest being used for all future FFTW calls using this plan.
- Old plans can be reused or even read from file: *wisdom*

FFTW: Installation

- Download library from the website and unpack
 - gzipped tar file
- **`./configure; make; make install`**
 - Probes the local environment
 - Compiles many small C object codes called *codelets*
 - User can provide non-standard compiler optimisation flags
 - Libraries (both static and dynamic) are then installed along with online documentation and header files
- Includes test suite
 - Very important for any numerical library
- Pre-installed with Scientific Linux

FFTW: Compiling code

- `gfortran fft_code.f -O3 -lfftw`
 - If using C, FFTW must be linked with `-lfftw -lm`
 - If the FFTW library is configured for both single and double precision, then link with `-lsfftw` and `-ldfftw`, respectively.

- Example FORTRAN code:

```
integer :: plan
integer, parameter :: n = 1024
complex :: in(n), out(n)
! plan the computation
call fftw_f77_create_plan(...)
! execute the plan
call fftw_f77_one(...)
```

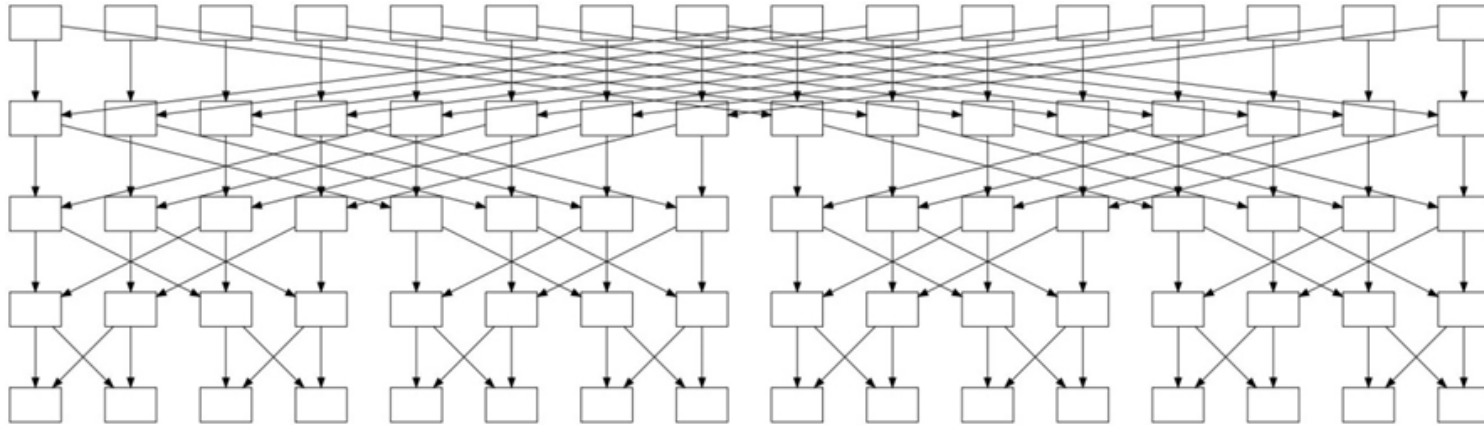
- NB: actual incantations are not given here as reading documentation is integral to utilising any numerical library

FFTW: Performance

- The FFTW homepage, www.fftw.org, details the performance of the library compared to proprietary FFTs on a wide range of platforms.
- The FFTW library is faster than any other portable FFT library
- Comparable with machine-specific libraries provided by vendors
- Performance results from <http://www.fftw.org/speed/>

Parallel 1D FFT (1/2)

- Parallelisation of a 1D FFT is hard
 - Combining of data requires a lot of inter-processor communication



- Typically $N \approx 100-200$ in many scientific codes e.g. materials chemistry – small amount of data
- Algorithm is hard to decompose
- Literature examples:

Franchetti, Voronenko, Püschel, “FFT Program Generation for Shared Memory: SMP and Multicore”, Paper presented at SC06, Tampa, FL

<http://sc06.supercomputing.org/schedule/pdf/pap169.pdf>

Tang et al, “A Framework for Low-Communication 1-D FFT”, SC12,
<https://software.intel.com/sites/default/files/bd/8b/fft-1d-framework.pdf>

Parallel 1D parallel FFT (2/2)

- Parallelisation works for large problems only ☹️
- Sensitive to contention (shared buses) ☹️
- Multicore chips with communications at cache level appear beneficial – might “be there” in a few years time
- Shows speedup, but not always “perfect” ☹️
- Presently: **1D FFT is an “expensive sum” of an array which is hard to parallelise**

FFTs in two dimensions

- What needs calculating for a 2D FFT:

$$\tilde{f}(k, l) = \sum_{y=1}^M \left\{ \sum_{x=1}^N \left[f(x, y) \exp \left(-2\pi i \frac{kx}{N} \right) \right] \exp \left(-2\pi i \frac{ly}{M} \right) \right\}$$

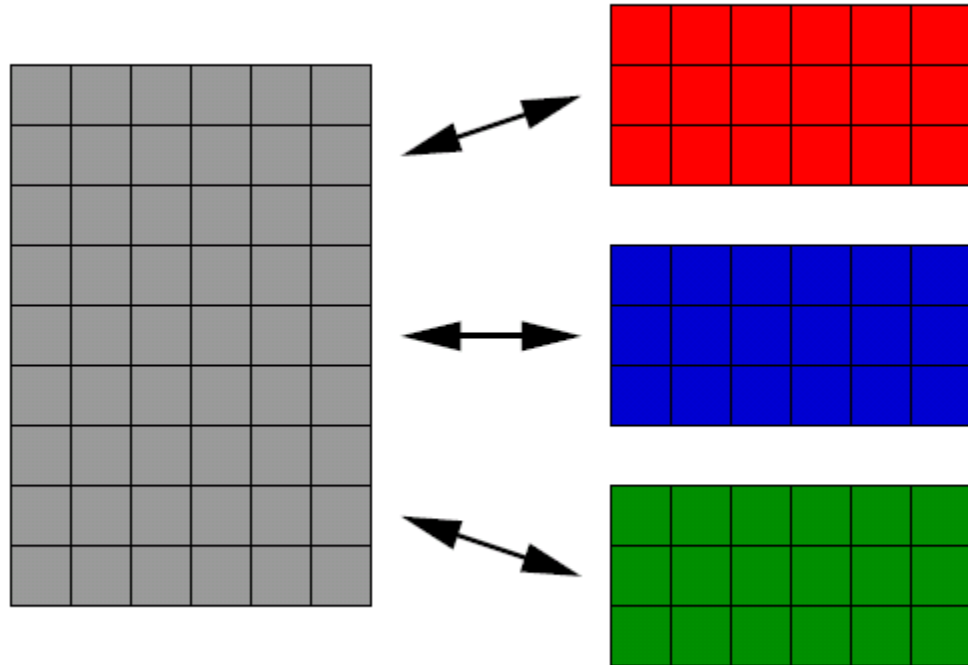
- Do it in a 2-step approach:

$$\hat{f}(k, y) \equiv \sum_{x=1}^N \left[f(x, y) \exp \left(-2\pi i \frac{kx}{N} \right) \right]$$

$$\tilde{f}(k, l) = \sum_{y=1}^M \left\{ \hat{f}(k, y) \exp \left(-2\pi i \frac{ly}{M} \right) \right\}$$

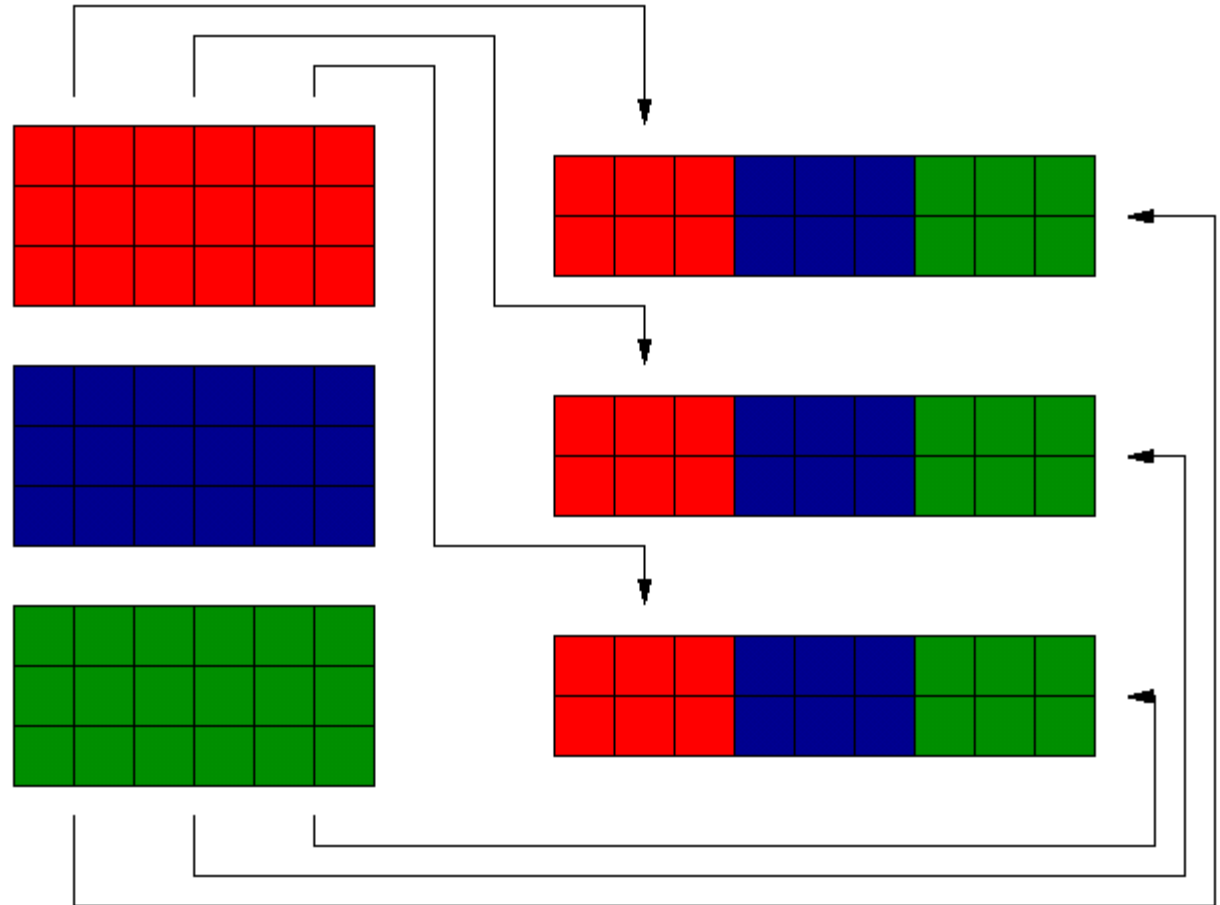
Distribute array onto 1D processor grid

- Example:
 - 6×9 array
 - 3 processors
 - Assuming row major order (C convention)
- Perform 1st FFT:
 - Each processor transforms 3 arrays of 6 elements
- What next?



Data transposition

- Divide up the array by columns for 2nd FFT
- Depending on FFT library simultaneous transpose can be advantageous (shown on figure)



Perform 2nd FFT

- What used to be the columns of the original array is now in row-major order 😊
- Do the 2nd FFT
 - In the example:
 - Each processor performs 2 FFTs of an array of length 9
- Rearrange data as required by following code
 - Examples:
 - Undoing the transpose
 - Redistributing data onto 2D grid
 - Sometimes: nothing needs done 😊

Fourier Transformation of a 3D array

- Definition of the Fourier Transformation of a 3D array $A_{x,y,z}$

$$\tilde{A}_{u,v,w} := \sum_{x=0}^{L-1} \sum_{y=0}^{M-1} \sum_{z=0}^{N-1} A_{x,y,z} \exp(-2\pi i \frac{wz}{N}) \exp(-2\pi i \frac{vy}{M}) \exp(-2\pi i \frac{ux}{L})$$

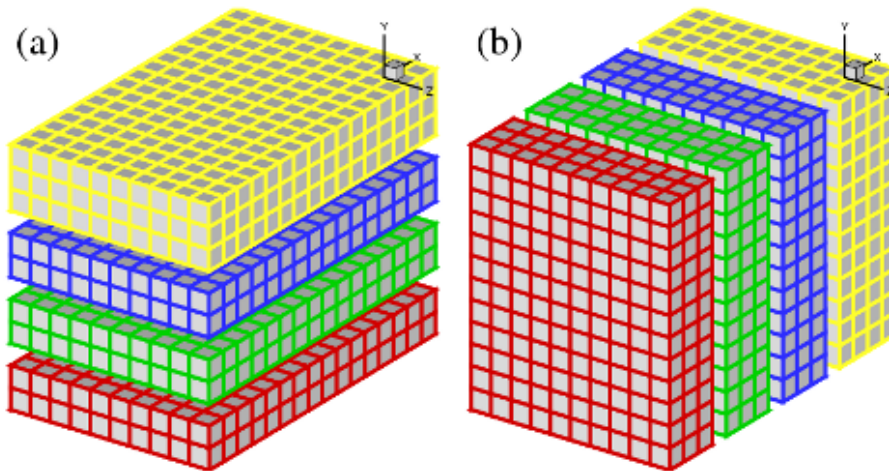
1st 1D FT along z

2nd 1D FT along y

3rd 1D FT along x

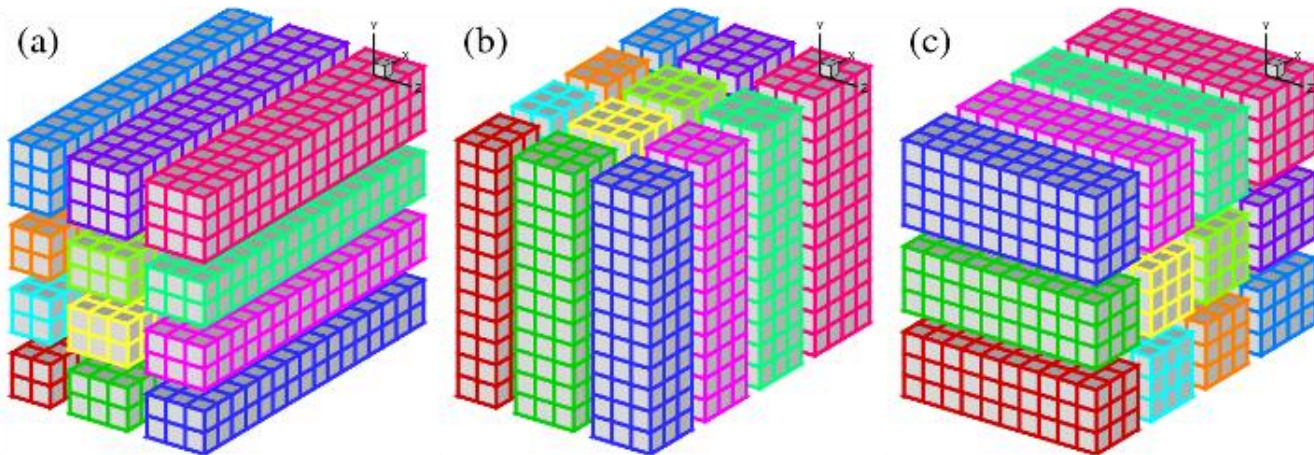
- Can be performed as three subsequent 1 dimensional FFTs

FFT Slab and Pencil decomposition



Slab: decomp in
Y and X directions
using 4 cores

Pencil: (a) X-, (b) Y-
and (c) Z-pencils
using 12 cores



Images from
2DECOMP&FFT library <http://www.2decomp.org/decomp.html>

FFT: Slab vs Pencil

- Slab
 - Pros: Simple with moderate amount of inter-processor communication
 - Cons: Limited to N procs for N^3 data
- Pencil
 - Pros: faster on massively parallel supercomputers (i.e. lots of cores)
 - Cons: More communications and now more complicated
- Pencil generally better with high core count but not so good for larger arrays on moderate number of cores
- Note: FFTW only does slab!

Summary of FFTs

- Parallelisation of an individual 1D FFT is hard
 - Presently works best for large problems
 - Recent advances in algorithms & hardware encouraging
- Multidimensional problems need to calculate many 1D FFTs
 - Parallelisable by distributing entire FFTs onto the processors and using a standard serial 1D FFT library
 - Requires redistributing the data between FFT dimensions
 - Need to think about decomposition (e.g. slab vs pencil)
- FFT can be used to reduce computational complexity of Fourier transform calculations from $O(n^2)$ to $O(n \log(n))$
 - Applications in signal processing, CFD, probability, etc.