Computational Methods (practice) - Lecture 1

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- Introduction & Resources
- Parallel computing and data parallel programming
- Sparse matrices, stencils & PDEs
- Example: (covariant) Laplacian
- Fourier tests
- Gauge invariance tests

Strategy

- Aim to give a discussion of key algorithms and topics in practical Lattice QCD simulation
  - Reasonable degree of rigour, without making this a formal mathematical approach.
  - Provide links to in depth papers and textbooks where appropriate
- *Will illustrate the lectures with practical examples based in Grid*
  - Perhaps a unique feature of this course - let me know what works and does not work !
  - Hope to convince you that lattice code can be small and expressive
- Intersperse discussion of computing/code with discussion of algorithms/physics
  - Hope this is reasonably entertaining
  - Reflects my prejudice that computing is most efficiently learned as required to solve problems
- C++ will be assumed

Assumed programming knowledge

- C++
  - operator overloading
  - template functions and classes - enables generic programming
  - inheritance and object orientation
  - Stroustroup

    https://www.amazon.co.uk/C-Programming-Language-Bjarne-Stroustrup/dp/0321563840

- "C" is so much smaller than C++ it is worth learning first: Kernigan and Ritchie

  https://www.amazon.co.uk/C-Programming-Language-2nd/dp/0131103628

  Several keywords in C++, such as "static" are often misnomers, dating to "C" usage

Why C++?

- Low level code is possible;
  you can take the compiler out of the way; intrinsics, inline asm etc...
- High level code is possible;
  objects and operator overloading allow to define a mathematical type system
  Very high level code with natural mathematical expressions
- Single code base can be powerful, portable and efficient
- Broad based compiler support and mature standards process
- CUDA, HIP, SYCL are all C++ based
- Veldhuizen, Expression Templates: *faster than fortran is possible*
- Templating: can write functions & objects (matrices, vectors) of any type multiple precisions, Real/Complex, matrix of matrix to capture tensorial structures of QFT

How many "abs" functions do we need?

```
#include <math.h>
double fabs(double x);
long double fabsl(long double x);
float fabsf(float x);
```

```
template<class t> t abs(t arg) ;
```

```
#include <stdlib.h>
int   abs(int i);
long labs(long i);
long long llabs(long long i);
```

Resources

- Computing:

https://www.amazon.co.uk/Feynman-Lectures-Computation-Frontiers-Physics/dp/0738202967

https://www.amazon.co.uk/Computer-Architecture-Quantitative-Approach-Kaufmann/dp/0128119055

- Grid:

www.github.com/paboyle/Grid

- Grid documentation:

https://github.com/paboyle/Grid/raw/develop/documentation/Grid.pdf

- Examples:

https://github.com/paboyle/Grid/tree/develop/examples

- More formal courses
- Tony Kennedy Nara lectures

https://arxiv.org/abs/hep-lat/0607038

- Iterative Methods for Sparse Linear Systems, Saad

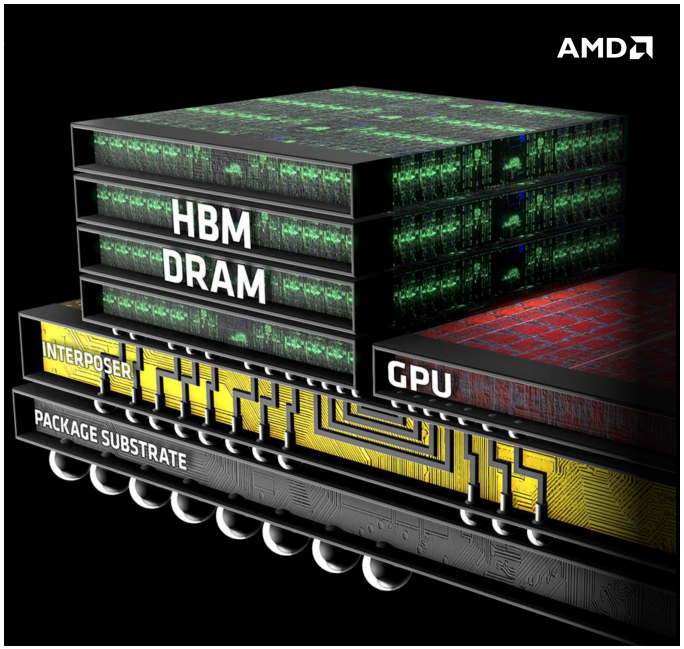
https://www-users.cse.umn.edu/~saad/IterMethBook_2ndEd.pdf

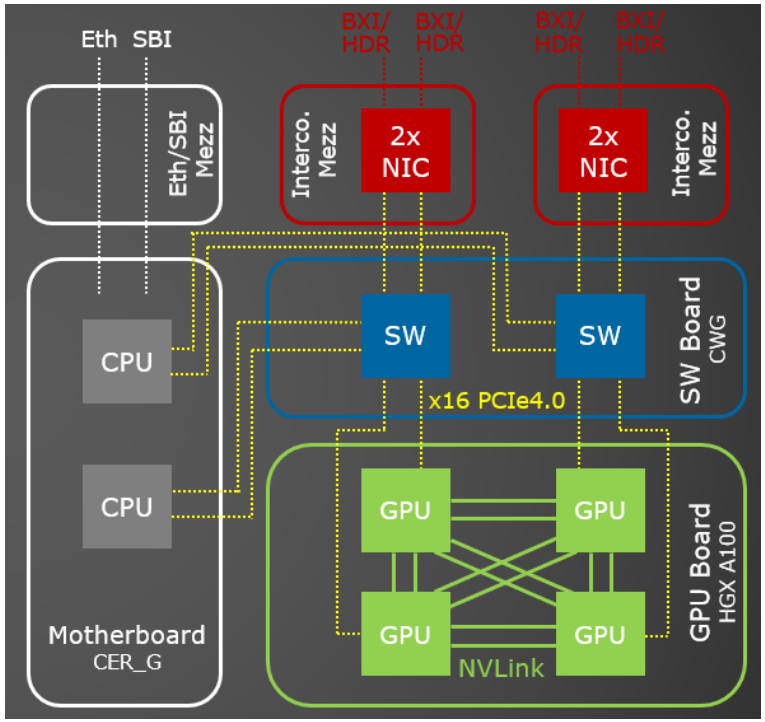
Parallel computing and data parallel programming

- Comprised of many computing nodes with programmed *message passing* between nodes
- Distributed memory MIMD architecture / loosely coupled multiprocessors
  - Complicated, cooperative access scheme for the data access (send/receive calls)
  - Standardised by: Message Passing Interface (MPI).
  - Predecessors: PVM.
  - Alternatives: UPC, PGAS `Array[node][offset]`
- Nodes themselves contain many layers of parallelism
  - Multiple cores of same type and multiple sockets
  - Accelerators ("vector" cores of different type in a plug-in device)
  - Two or more distinct memory spaces and instruction sets in same programme
  - Multiple vendor supported APIs: CUDA/Nvidia; HIP/AMD; OneAPI/Intel
  - Portability barrier(!)

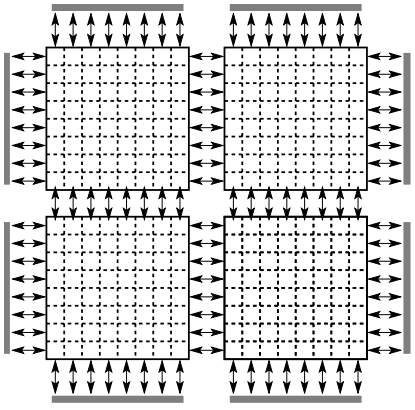
Parallel computing and data parallel programming

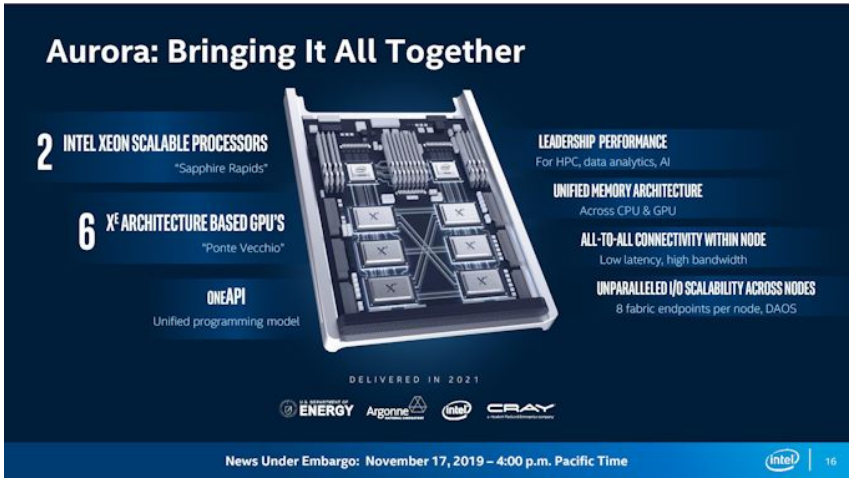
- **Modern supercomputers are increasingly difficult to programme**
  - This is not the way things used to be, nor in my view the way things should be
- Basic physics dictates that large computers are massively parallel and only locally well interconnected
  - Wires can be long and slow or short and fast (aspect ratio dictates RC delay)
  - Chips must be locally divided into cores
  - "Memory" can be small and fast OR big and slow $\Rightarrow$ caches
  - 3D "Memory", HBM and hierarchical memory
  - Interconnect is over a few large high speed wires (or optical transceivers).





Parallel computing and data parallel programming





- 112 nodes of ATOS Sequana XH2000 with 4x A100-40 GPUs per node
- 2x AMD Rome 7H12 CPUs
- 1TB DDR per node
- 4 x HDR-200 infiniband per node

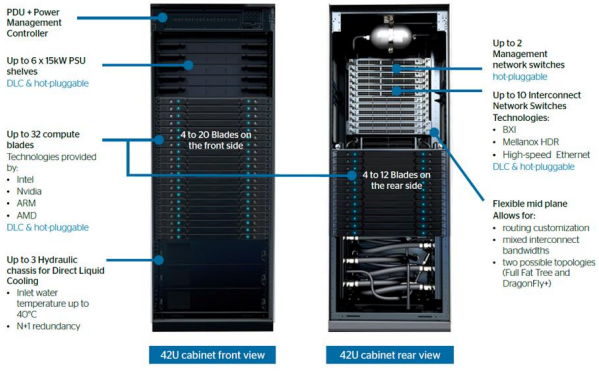


Figure 2-2 BullSequana XH2000 rack

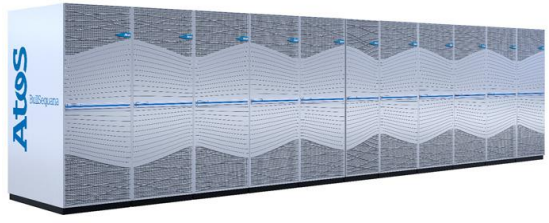


Figure 2-1 BullSequana XH2000 Integrated Supercomputer

Forthcoming Exascale computers

Frontier AMD CPU, AMD GPU; HIP

Perlmutter AMD CPU, Nvidia GPU; CUDA

Aurora Intel CPU, Intel GPU; SYCL

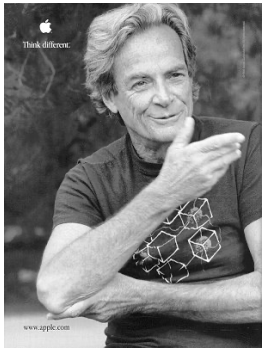
Summit IBM CPU, Nvidia GPU; CUDA

+ CPU computing is also *not* going away

Parallel computing and data parallel programming

- How to portably target highly parallel hardware ?
  - Easiest if the syntax is high level, and then broken up under an interface
  - Data parallel *used* to mean more than concurrently executed loop bodies – treat entire arrays as objects
  - "Borrow" concepts from the *Connection Machine*

CM-2



- https://longnow.org/essays/richard-feynman-connection-machine/
- https://people.csail.mit.edu/bradley/cm5docs/CMFortranProgrammingGuide.pdf
- Compare with QDP++
- HPF failed due to poor performance over MPI: systematic stencil operation assistance
  - *PGAS will probably fail for the same reasons!*
- Never break a high level operation into a specific ordering and expect language to reorder Entropy in action! Preserve higher level information

High level data parallelism

- At the highest level deal with a distributed array across a multi-node computer as an aggregate object
  - Periodic CSHIFT / Dirichlet EOSHIFT primitives
  - Conformable array operations on arrays of identically laid out data
    - c.f. F90 syntax array wildcarding/slicing
  - Predicated data parallel operation (where)

- High Performance Fortran was a failure due to MPI latency
  - Introduce additional, lower-level support for PDE stencil operations & halo exchange.

- Use C++ opaque containers for distributed arrays
  - Operator overloading leaves expressions “natural”
  - (compact C++11, 200 LoC) expression template engine keeps site local expressions optimized.

- Supports CPU w/ SIMD, CUDA, SyCL 2020, HIP compilation targets
  - Device data motion uses either software cache or unified virtual memory

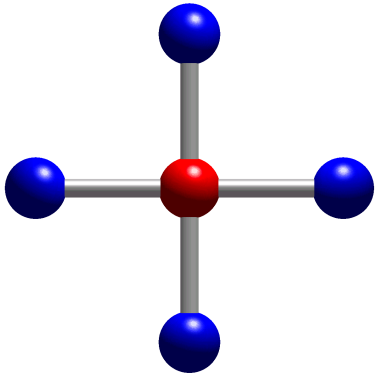
```
A=B*C+Cshift(D,1,Xdir);

face = (mod(coor,Block[mu]) == 0) ;

projected= where(face==1,sp_proj,projected);
```

Sparse matrices, stencils & PDEs

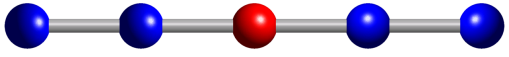
- Encode differential operators as discrete finite difference derivatives
- Think of as sparse matrices - typically band diagonal

$$M(x,y) = \frac{\delta_{x+\mu,y} + \delta_{x-\mu,y} - 2\delta_{x,y}}{a^2}$$

- In typicaly PDE usage, discretisation schemes can be encoded via coefficients and a *stencil*
- The *stencil* is a geometric shape encoding the set of points y that contribute to the operator at point x
- This is translationally invariant and characteristic of a discretisation scheme.
- Naive Laplacian and Wilson Fermions have a $2N_d + 1$ point stencil
- Improved staggered Fermions n discretisations have a $4N_d + 1$ point stencil
- Fourier transformation $\Rightarrow$ phase factor on each term in the stencil defines the lattice Feynman rules
- More non-local actions allow higher order improvement (classical/perturbative/NP)
  c.f. Hamber-Wu, Naik terms.



2D Wilson stencil



Higher order derivative stencil

$$c_1(e^{ip_\mu} - e^{-ip_\mu}) + c_2(e^{i2p_\mu} - e^{-i2p_\mu}) \rightarrow ip_\mu + O(p_\mu^5)$$

Grids primitives (see documentation)

- Common QCD discretisations suggest we can construct most operations with
  - N-dimensional grids
  - Shifting along coordinate axes
  - Gauge covariant of shifting fields
  - Cartesian stencil operators along axes only
  - Generic stencil operators within some taxi-cab distance
  - Site local arithmetic: matrix/vector/scalar addition, subtraction, multiplication, math library functions
  - Reductions: Inner-product, norm2, volume sum, slice summing (N-1 dim)
  - N-dim FFT
  - BlockProjection/Promotion between coarse and fine grids

Example: Free and covariant Laplacian

https://www.github.com/paboyle/Grid/examples/Example_Laplacian.cc

- Base class *defines an interface*.
- Specific derived classes inherit and implement this interface differently
- Algorithms deal with the base class and work with all derived operators

```
////////////////////////////////////////////////////////////////////////////////////////
// Grid/algorithms/SparseMatrix.h: Interface defining general sparse matrix, such as a Fermion action
////////////////////////////////////////////////////////////////////////////////////////
template<class Field> class SparseMatrixBase {
public:
  virtual GridBase *Grid(void) =0;

  virtual void  M    (const Field &in, Field &out)=0;
  virtual void  Mdag (const Field &in, Field &out)=0;
  virtual void  MdagM(const Field &in, Field &out) {
    Field tmp (in.Grid());
    M(in,tmp);
    Mdag(tmp,out);
  }
};
```

Example: Free Laplacian (low performance)

Introduce free field Cshift based Laplacian:

```
template<class Field> class FreeLaplacianCshift : public SparseMatrixBase<Field>
{
public:
  GridBase *grid;
  FreeLaplacianCshift(GridBase *_grid)
  {
    grid=_grid;
  };
  virtual GridBase *Grid(void) { return grid; };

  virtual void  M    (const Field &in, Field &out)
  {
    out = Zero();
    for(int mu=0;mu<Nd-1;mu++) {
      out = out + Cshift(in,mu,1) + Cshift(in,mu,-1) - 2.0 * in;
    }
  };
  virtual void  Mdag (const Field &in, Field &out) { M(in,out);}; // Laplacian is hermitian
};
```

Example: Covariant Laplacian (low performance)

```
template<class Gimpl,class Field> class CovariantLaplacianCshift : public SparseMatrixBase<Field>
{
  INHERIT_GIMPL_TYPES(Gimpl);

  GridBase *grid;
  GaugeField U;

  CovariantLaplacianCshift(GaugeField &_U)    :    grid(_U.Grid()),    U(_U) {  };

  virtual void  M    (const Field &in, Field &out)
  {
    out=Zero();
    for(int mu=0;mu<Nd-1;mu++) {
      GaugeLinkField Umu = PeekIndex<LorentzIndex>(U, mu); // NB: Inefficent
      out = out + Gimpl::CovShiftForward(Umu,mu,in);
      out = out + Gimpl::CovShiftBackward(Umu,mu,in);
      out = out - 2.0*in;
    }
  };
  virtual void  Mdag (const Field &in, Field &out) { M(in,out);}; // Laplacian is hermitian
};
```

- The covariant shift is passed in through a policy template parameter class
- Knowledge of boundary conditions is external: we've written Laplacian code that works for periodic *and* charge conjugation boundary conditions
- Wilson loops, Gauge actions, Fermion actions in Grid follow similar design ideas

Fourier test

```
std:: cout << " Test A: compare in free Field to \"Feynman rule\" / Convolution theorem " <<std::endl;

std::vector<int> dim_mask({1,1,1,0}); // 3d FFT

FFT theFFT(&Grid);

Field out(&Grid), F_out(&Grid), F_in(&Grid);

// FFT the random input vector
theFFT.FFT_dim_mask(F_in,in,dim_mask,FFT::forward);

// Convolution theorem: multiply by Fourier representation of (discrete) Laplacian to apply diff op
LatticeComplexD    lap(&Grid); lap = Zero();
LatticeComplexD    kmu(&Grid);

for(int mu=0;mu<3;mu++) {

  RealD TwoPiL =  M_PI * 2.0/ latt_size[mu];

  LatticeCoordinate(kmu,mu);
  kmu = TwoPiL * kmu;

  // (e^ik_mu + e^-ik_mu - 2) = 2( cos kmu - 1) ~ 2 (1 - k_mu^2/2 -1 ) =k_mu^2 + O(k^4)
  lap = lap + 2.0*cos(kmu) - 2.0;

}
F_out = lap * F_in;

// Inverse FFT the result
theFFT.FFT_dim_mask(out,F_out,dim_mask,FFT::backward);

std::cout<<"Fourier xformed (in)             "<<norm2(F_in)<<std::endl;
std::cout<<"Fourier xformed Laplacian x (in) "<<norm2(F_out)<<std::endl;

std::cout<<"Momentum space Laplacian application  "<< norm2(out)<<std::endl;
std::cout<<"Stencil Laplacian application         "<< norm2(out_CLcs)<<std::endl;

diff = out_CLcs - out;
std::cout<<"diff "<< norm2(diff)<<std::endl;
```

Output

- Compare to application in momentum space
  - Textbook exercise; use to verify code on unit gauge + a random gauge transform of unit gauge
  - Every Fermion action in Grid knows its own lattice Feynman rule and can *self test* the free propagator
  - In addition to regression to other code bases such as Chroma, Bagel or CPS
  - Add gauge covariance and tests with all Gauge links being highly non-trivial are possible

```
*****************************************************************
 Test A: compare in free Field to "Feynman rule"
*****************************************************************
Fourier xformed (in)             1.25907e+07
Fourier xformed Laplacian x (in) 5.25498e+08
Momentum space Laplacian application  1.02636e+06
Stencil Laplacian application         1.02636e+06
diff 1.0201e-25
```

Gauge invariance test

```
std:: cout << "*****************************************************************" <<std::endl;
std:: cout << " Test B: gauge covariance  " <<std::endl;
std:: cout << "*****************************************************************" <<std::endl;

LatticeGaugeField     U_GT(&Grid); // Gauge transformed field
LatticeColourMatrix   g(&Grid);   // local Gauge xform matrix

U_GT = U;
// Make a random xform to teh gauge field
SU<Nc>::RandomGaugeTransform(RNG,U_GT,g); // Unit gauge

Field in_GT(&Grid);
Field out_GT(&Grid);

Field out_CLcs_GT(&Grid);
Field out_CLst_GT(&Grid);

CovariantLaplacianCshift <PeriodicGimplR,Field> CLcs_GT(U_GT);
CovariantLaplacianStencil<PeriodicGimplR,Field> CLst_GT(U_GT);

in_GT  = g*in;
out_GT = g*out_FLcs;

// Check M^GT_xy in_GT = g(x) M_xy g^dag(y) g(y) in = g(x) out(x)
CLcs_GT.M(in_GT,out_CLcs_GT);
CLst_GT.M(in_GT,out_CLst_GT);

diff = out_CLcs_GT - out_GT;
std:: cout << " Difference between Gauge xformed result and covariant Cshift Laplacian in xformed gauge  = " <<norm2(diff)<<std::endl;

diff = out_CLst_GT - out_GT;
std:: cout << " Difference between Gauge xformed result and covariant Stencil Laplacian in xformed gauge  = " <<norm2(diff)<<std::endl;
std:: cout << "-----------------------------------------------------" <<std::endl;
```

Output

```
*****************************************************************
 Test B: gauge covariance
*****************************************************************
 Difference between Gauge xformed result and covariant Cshift Laplacian in xformed gauge  = 7.28706e-23
 Difference between Gauge xformed result and covariant Stencil Laplacian in xformed gauge  = 7.28985e-23
-----------------------------------------------------------
```

- Covariance of operators is an reasonably strong check
  Many mistakes will break the gauge invariance
- Hadronic correlation functions should be gauge invariant (ignore gauge fixed procedures)
- Variations of this test are a common "test weapon of choice"
  A necessary **but not sufficient** condition for correctness, loved by older LQCD scientists
- The above two tests combined - correctness on a random gauge transform of free field prove the operator behaves as intended with non-unit random gauge links on every variable: **a strong check**

Compare different implementations

```
FreeLaplacianCshift<Field>  FLcs(&Grid);
FreeLaplacianStencil<Field> FLst(&Grid);

LatticeGaugeField U(&Grid);
SU<Nc>::ColdConfiguration(RNG,U);

CovariantLaplacianCshift <PeriodicGimplR,Field> CLcs(U);
CovariantLaplacianStencil<PeriodicGimplR,Field> CLst(U);

std:: cout << " Test C: consistency of four different Laplacian implementations " <<std::endl;

Field in(&Grid); gaussian(RNG,in);

std:: cout << " Input test vector " <<norm2(in)<<std::endl;

Field out_FLcs(&Grid);  Field out_FLst(&Grid);
Field out_CLcs(&Grid);  Field out_CLst(&Grid);
Field diff(&Grid);

FLcs.M(in,out_FLcs);
FLst.M(in,out_FLst);
CLcs.M(in,out_CLcs);
CLst.M(in,out_CLst);
std:: cout << "-----------------------------------------------------------" <<std::endl;
std:: cout << " Free cshift  output vector " <<norm2(out_FLcs)<<std::endl;
std:: cout << " Free stencil output vector " <<norm2(out_FLst)<<std::endl;
std:: cout << " Cov  cshift  output vector " <<norm2(out_CLcs)<<std::endl;
std:: cout << " Cov  stencil output vector " <<norm2(out_CLst)<<std::endl;
std:: cout << "-----------------------------------------------------------" <<std::endl;

diff = out_FLcs - out_FLst;
std:: cout << " Difference between free Cshift Laplacian and free Stencil Laplacian      = " <<norm2(diff)<<std::endl;

diff = out_FLcs - out_CLcs;
std:: cout << " Difference between free Cshift Laplacian and covariant Cshift Laplacian  = " <<norm2(diff)<<std::endl;

diff = out_FLcs - out_CLst;
std:: cout << " Difference between free Cshift Laplacian and covariant Stencil Laplacian = " <<norm2(diff)<<std::endl;
std:: cout << "-----------------------------------------------------------" <<std::endl;
```

Output

```
*****************************************************************
 Test C: consistency of four different Laplacian implementations
*****************************************************************
 Input test vector 24591.2
---------------------------------------------------------
 Free cshift  output vector 1.02636e+06
 Free stencil output vector 1.02636e+06
 Cov  cshift  output vector 1.02636e+06
 Cov  stencil output vector 1.02636e+06
---------------------------------------------------------
 Difference between free Cshift Laplacian and free Stencil Laplacian      = 2.2926e-26
 Difference between free Cshift Laplacian and covariant Cshift Laplacian  = 0
 Difference between free Cshift Laplacian and covariant Stencil Laplacian = 2.2926e-26
---------------------------------------------------------
```

- Stencil vs. Cshift based cross checked.
- Free and covariant implementations on unit gauge
- Can also compare different code bases (Chroma/CPS/Bagel/QUDA etc...)
  - Weak to a common error (e.g. copy the same Dirac basis?), not scientifically independent
- The Wilson and DWF type actions in Grid have been tested in the above fashion
- Caution: the Clover field strengh is identically zero in a transform of free field

Exercise

- Obtain and compile Grid;
- Read and run the example

```
git clone https://www.github.com/paboyle/Grid
cd Grid
./bootstrap.sh
mkdir build
cd build
../configure --enable-simd=GEN --enable-debug
make -j 8
cd examples
./Example_Laplacian
```