HMC, high level structures and architecture support in Grid

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in collaboration with

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GRID library

Started from Peter’s effort to design a modern C++ library for Cartesian mesh problems

Design goals
- performance portability
- zero code replication

Grid github pages github.com/paboyle/Grid
(partial) documentation paboyle.github.io/Grid/
CI: Travis, TeamCity https://ci.cliath.ph.ed.ac.uk/

Source code: C++11, autotools

+ HADRONS physics measurement framework based on Grid (A. Portelli)
Intense work in progress, production stage next year

Harness the power of generic programming

- Define algorithms for generic types
- Templates & template metaprogramming
- Define general interfaces and let the compiler do the hard job
- Basic types will mask the architecture from high level classes
- Enters C++11
  - type inference
  - new standard library, metaprogramming improvements
  - type traits
  - variadic templates
  - ...
- Write code once!

vSIMD, basic portable vector types

Define performant classes `vRealF, vRealD, vComplexF, vComplexD`.

Here very simplified, actual implementation use extensively C++11 type traits.

```
#if defined (AVX1) || defined (AVX2)
         typedef __m256 SIMD_Ftype;
#endif
#if defined (SSE2)
         typedef __m128 SIMD_Ftype;
#endif
#if defined (AVX512)
         typedef __m512 SIMD_Ftype;
#endif
template <class Scalar_type, class Vector_type>
class Grid_simd {
         Vector_type v;
         // Define arithmetic operators
         friend inline vRealD operator + (vRealD a, vRealD b);
         friend inline vRealD operator - (vRealD a, vRealD b);
         friend inline vRealD operator * (vRealD a, vRealD b);
         friend inline vRealD operator / (vRealD a, vRealD b);
         static int Nsimd(void) { return sizeof(Vector_type)/sizeof(Scalar_type);
}
typedef Grid_simd<float, SIMD_Ftype> vRealF;
```

GRID library: architecture support

Current support

- SSE4.2
- AVX, AVX2 (e.g. Intel Haswell, Broadwell, AMD Ryzen)
- AVX512F (Intel KNL, Skylake)
- QPX (BlueGene/Q), experimental
- NEON ARMv8 (on the way, thanks to Nils Meyer from Regensburg University)
- Generic vector width support

Plans for

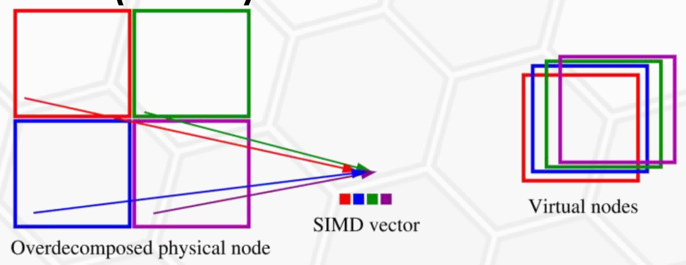
- CUDA threads (Nvidia GPUs) (Alexander Wennersteen & ECP collaboration)
- ARM SVE (Scalable Vector Extensions, Fujitsu post-K)

Each file is O(500) lines of code describing the lowest level operations on the vector types

- Real/Complex algebra
- Load/Store, vstream
- Rotations
- Permutations
- Precision change

GRID parallel library

- Geometrically decompose cartesian arrays across nodes (MPI)
- Subdivide node volume into smaller virtual nodes
- Spread virtual nodes across SIMD lanes
- Use OpenMP+MPI+SIMD to process *conformable array* operations
- Same instructions executed on many nodes, each node operates on `Nsimd` virtual nodes
- Conclusion: modify data layout to align data parallel operations to SIMD hardware
- Conformable array operations are simple and vectorise perfectly



Grid data parallel template library

- Opaque C++11 containers hide data layout from user
- Automatically transform layout of arrays of mathematical objects using vSIMD scalar, vector, matrix, higher rank tensors.

General linear algebra with vector types

```
vRealF, vRealD, vComplexF, vComplexD

template<class vtype> class iScalar
{
      vtype _internal;
};
template<class vtype,int N> class iVector
{
      vtype _internal[N];
};
template<class vtype,int N> class iMatrix
{
      vtype _internal[N][N];
};
```

- Defines matrix, vector, scalar site operations
- Internal type can be SIMD vectors *or* scalars

```
LatticeColourMatrix A(Grid);
LatticeColourMatrix B(Grid);
LatticeColourMatrix C(Grid);
LatticeColourMatrix dC_dy(Grid);
C = A*B;
const int Ydim = 1;
dC_dy = 0.5*Cshift(C,Ydim, 1 ) - 0.5*Cshift(C,Ydim,-1 );
```

- *High-level* data parallel code gets 65% of peak on AVX2
- Single data parallelism model targets BOTH SIMD and threads efficiently.

QCD types example:

```
template<typename vtype> using
iLorentzColourMatrix =
iVector<iScalar<iMatrix<vtype, Nc> >, Nd > ;
```

GRID library: HMC summary

- Actions
  - Gauge: Wilson, Symanzik, Iwasaki, RBC, DBW2, generic Plaquete + Rectangle
  - Fermion: Two Flavours, One Flavour (RHMC), Two Flavours Ratio, One Flavour Ratio. All with the EO variant.
  - Kernels: Wilson, Wilson TM, generalised DWF (Shamir, Scaled Shamir, Mobius, Zmobius, Overlap, …)
  - Scalar Fields
- Integrators: Leapfrog, 2nd order minimum-norm (Omelyan), force gradient, + implicit versions
- Fermion representations
  - Fundamental, Adjoint, Two-index symmetric, Two-index antisymmetric, and all possible mixing of these. Any number of colours. All fermionic actions are compatible.
- Stout smeared evolution with APE kernel (for SU(3) fields). Any action can be smeared.
- Serialisation: XML, JSON
- Algorithms: GHMC, RMHMC, LAHMC, density of states LLR easily implemented
- File Formats: Binary, NERSC, ILDG, SCIDAC (for confs). MPI-IO for efficient parallel IO

Some features inherited by IroIro++

GRID library: HMC design

Need to support a large variety of actions, e.g.

- Scalar field theories
- Fermions in different representations (in any combination)
- Different algorithms (HMC, RMHMC, LAHMC, DoS)

Abstract away invariant concepts by templating

```
template <class Implementation,
          template <typename, typename, typename> class Integrator,
          class RepresentationsPolicy = NoHirep, class ReaderClass = XmlReader>
class HMCWrapperTemplate: public HMCRunnerBase<ReaderClass>


template <class FieldImplementation, class SmearingPolicy, class RepresentationPolicy>
class Integrator
```

GRID library: HMC design

```
template <class Implementation,
          template <typename, typename, typename> class Integrator,
          class RepresentationsPolicy = NoHirep, class ReaderClass = XmlReader>
class HMCWrapperTemplate: public HMCRunnerBase<ReaderClass>
```

Implementation

Boundary conditions
Field types
Momenta generation
Field update
Force projection

Representation

Update representation
Force Algebra projection
Representation to Fundamental projection

C++11 `std::tuples`
The action set is a collection of actions
Need to manage different types
Dispatches the correct function when requested

GRID library: HMC highest level design

User point of view, three usage models:

- Pure C++ code
- Pure C++ and serialisation (all parameter classes are serializable), XML or JSON
- Full control via XML using factories (highest level ~20 lines of code)

Module structure + resources class

GRID library: pure C++

```cpp
int main(int argc, char **argv) {
using namespace Grid;
using namespace Grid::QCD;

Grid_init(&argc, &argv); GridLogLayout();

// Typedefs to simplify notation
typedef GenericHMCRunner<MinimumNorm2> HMCWrapper;
HMCWrapper TheHMC;

// Grid from the command line
TheHMC.Resources.AddFourDimGrid("gauge");
// Possibile to create the module by hand
// hardcoding parameters or using a Reader

// Checkpointer definition
CheckpointerParameters CPparams;
CPparams.config_prefix = "ckpoint_lat";
CPparams.rng_prefix = "ckpoint_rng";
CPparams.saveInterval = 1;
CPparams.format = "IEEE64BIG";
TheHMC.Resources.LoadNerscCheckpointer(CPparams);

RNGModuleParameters RNGpar;
RNGpar.serial_seeds = "1 2 3 4 5";
RNGpar.parallel_seeds = "6 7 8 9 10";
TheHMC.Resources.SetRNGSeeds(RNGpar);

// Construct observables
typedef PlaquetteMod<HMCWrapper::ImplPolicy> PlaqObs;
typedef TopologicalChargeMod<HMCWrapper::ImplPolicy> QObs;
TheHMC.Resources.AddObservable<PlaqObs>();
TheHMC.Resources.AddObservable<QObs>();
/////////////////////////////////////////////////////////////
// Collect actions
RealD beta = 5.6 ;
WilsonGaugeActionR Waction(beta);
ActionLevel<HMCWrapper::Field> Level1(1);
Level1.push_back(&Waction);
TheHMC.TheAction.push_back(Level1);
/////////////////////////////////////////////////////////////

// HMC parameters are serialisable
TheHMC.Parameters.MD.MDsteps = 20;
TheHMC.Parameters.MD.trajL = 1.0;

TheHMC.ReadCommandLine(argc, argv);
TheHMC.Run();
Grid_finalize();
} // main
```

GRID library: pure C++ and serializers

```
namespace Grid{
struct FermionParameters: Serializable {
GRID_SERIALIZABLE_CLASS_MEMBERS(FermionParameters,
         int, Ls,
         double, mass,
         double, M5,
         double, b,
         double, c,
         double, StoppingCondition,
         int, MaxCGIterations,
         bool, ApplySmearing);
};


struct MobiusHMCParameters: Serializable {
GRID_SERIALIZABLE_CLASS_MEMBERS(MobiusHMCParameters,
         double, gauge_beta,
         FermionParameters, Mobius)
```

```
typedef Grid::JSONReader JSONSerialiser;
typedef Grid::XMLReader XMLSerialiser;
HMCWrapper TheHMC;
JSONSerialiser Reader(TheHMC.ParameterFile);

MobiusHMCParameters MyParams(Reader);
```

Summary

Architecture support

- Wide variety of architectures
- Fairly easy implementation: new vector architecture support essentially needs just reading the ISA
- GPU support, work in progress using CUDA by Alexander Wennersteen + ECP collaboration

Grid HMC fairly flexible

- Accommodates a variety of theories/algorithms
- Mixed representations implemented by aggregating types, `std::tuples`

Currently number of dimensions and colours are hardcoded
Plan: create "LatticeTheory" classes that define these and template the implementations to mix gauge theories.

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