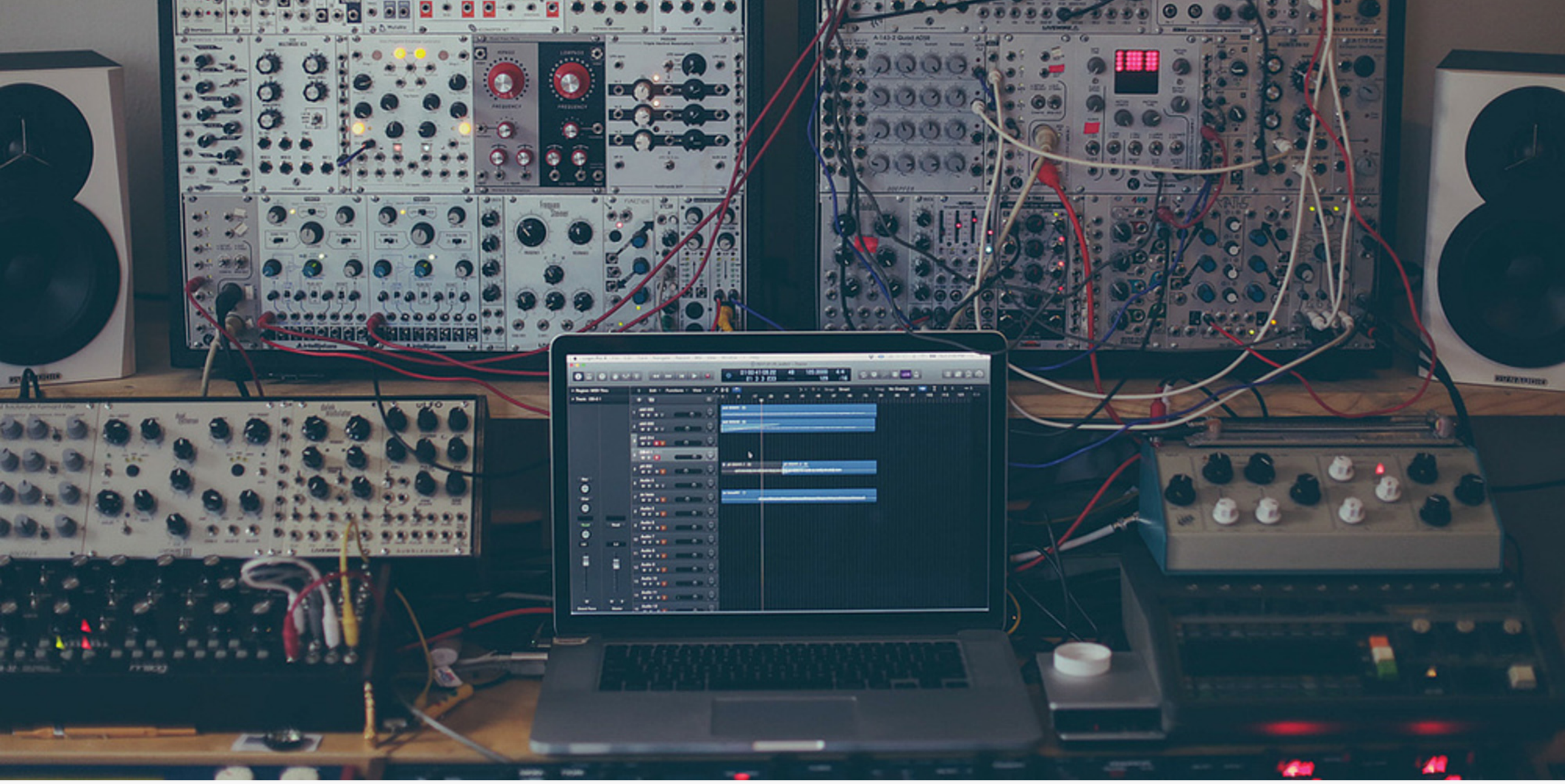

Hadrons: a Grid-powered measurement workflow management system

Antonin Portelli

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Lattice 2019 - Wuhan, China

erc

Centre for Theoretical Physics · Higgs

The University of Edinburgh

THE UNIVERSITY *of* EDINBURGH

Photo: Alex Kacha for Sound on Sound

- Developers: Boyle, Cossu, Filaci, Portelli, Yamaguchi
- + Richtman, O'Haigan, Kettle, Erben, Marshall, Murphy, Jung, Lehner

Develop branch: excellent multicore CPU performance

- Contains functionality equivalent to QMP, QIO, QDP++, and much of Chroma
- SU(N), U(1), multiple fermion representations
- Gauge evolution: HMC, RHMC, EOFA
- Wilson, Clover, Domain wall, Mobius, + various 5D overlap
  - Improved staggered valence action
- Multiple solvers
  - Mixed precision Krylov solvers (CG, GMRES, BiCGstab …)
  - Block solvers
  - Polynomial preconditioned Lanczos & deflation
  - Experimental multigrid
- Split Grids for valence solves - avoid communication
    - NB: Not the same as trivial parallelism:
      - Eigenvectors held globally, deflate many RHS
      - Solves are local. 3x gain on Cori

feature/gpu-port

- Aim to target multiple accelerators (Nvidia, AMD, Intel Aurora system)

- Presently compile all C++ files through NVCC (no .cu files)
  - Minimise vendor specific code to a few macros
    - Study HIP, OpenMP 5.0, SyCL options for other targets
  - Assume host and device have a unified memory space (UVM, SVM)

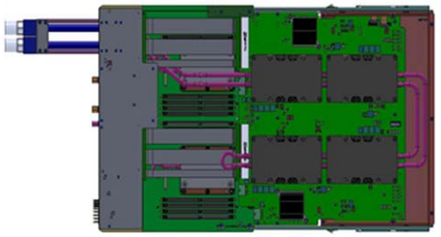
- (recent) Single source high performance kernels:
  - same kernel gives good performance on GPU *and* CPU

- All Fermion operators now accelerated
  - Wilson, Wilson5D, Improved Staggered
  - 5D Mobius terms also

- Entire CG runs on GPU. Full (R)HMC next target.

- Intra node GPU-GPU communication uses NVlink ; multi node under test

HPE ICE XA780i Quad Volta blade
24^4 5D single precision Wilson operator
1GPU 1.45 TF/s
4GPU 4.5 TF/s



Lattice measurements

- In QCD basically:
  Solver - Propagators - Contractions

- More and more involved:
  Deflation, AMA, 4-pt functions…

Things I did not want to repeat

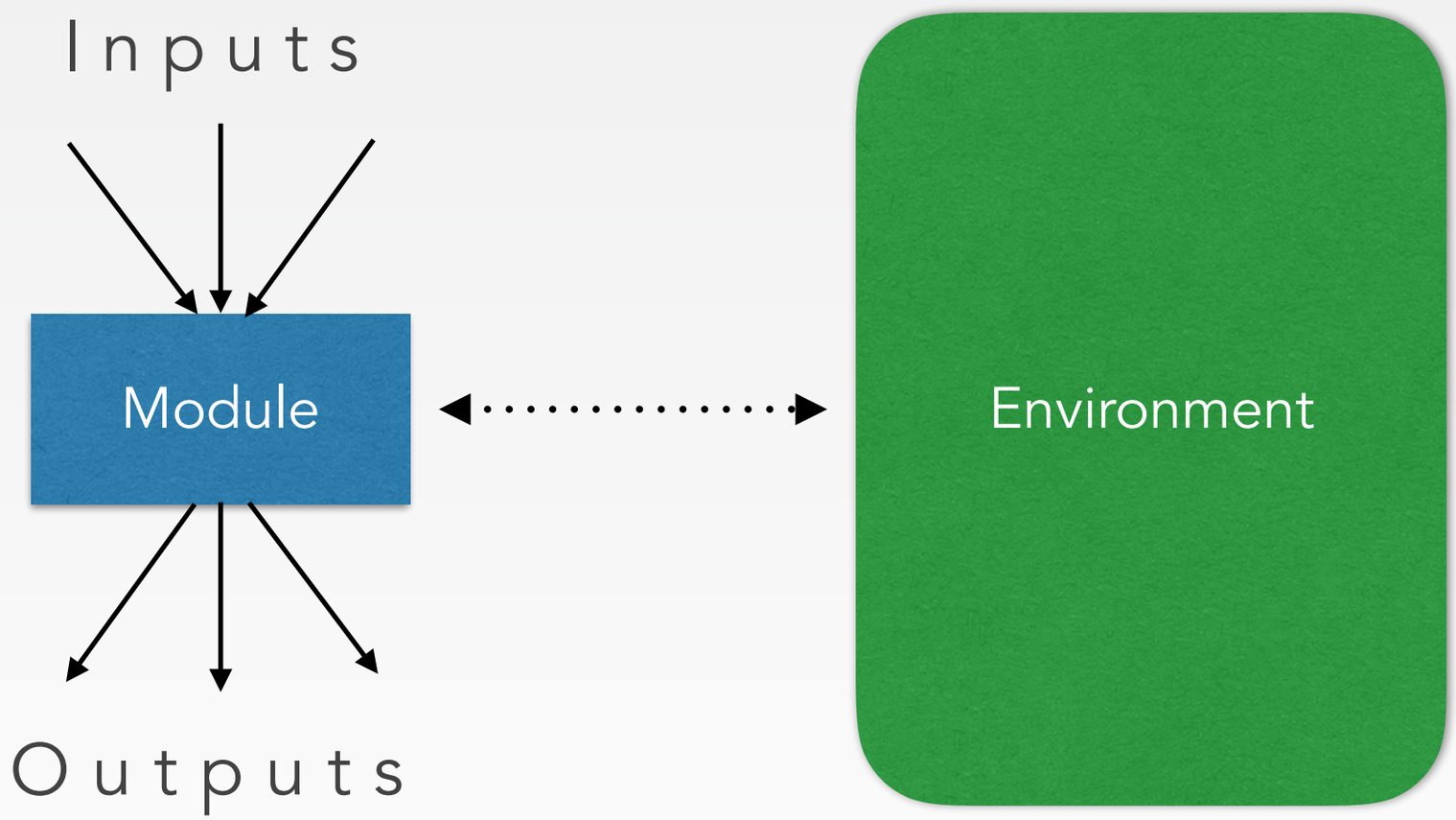
(no hard feelings, just trying to improve 🙂)

- **Very complicated inputs.**
  (100k lines XML files, machine generated inputs)
- **Very rigid programs.**
  (lots of global variables scattered in the program)
- **No safety net.**
  (dependency between steps, memory consumption)

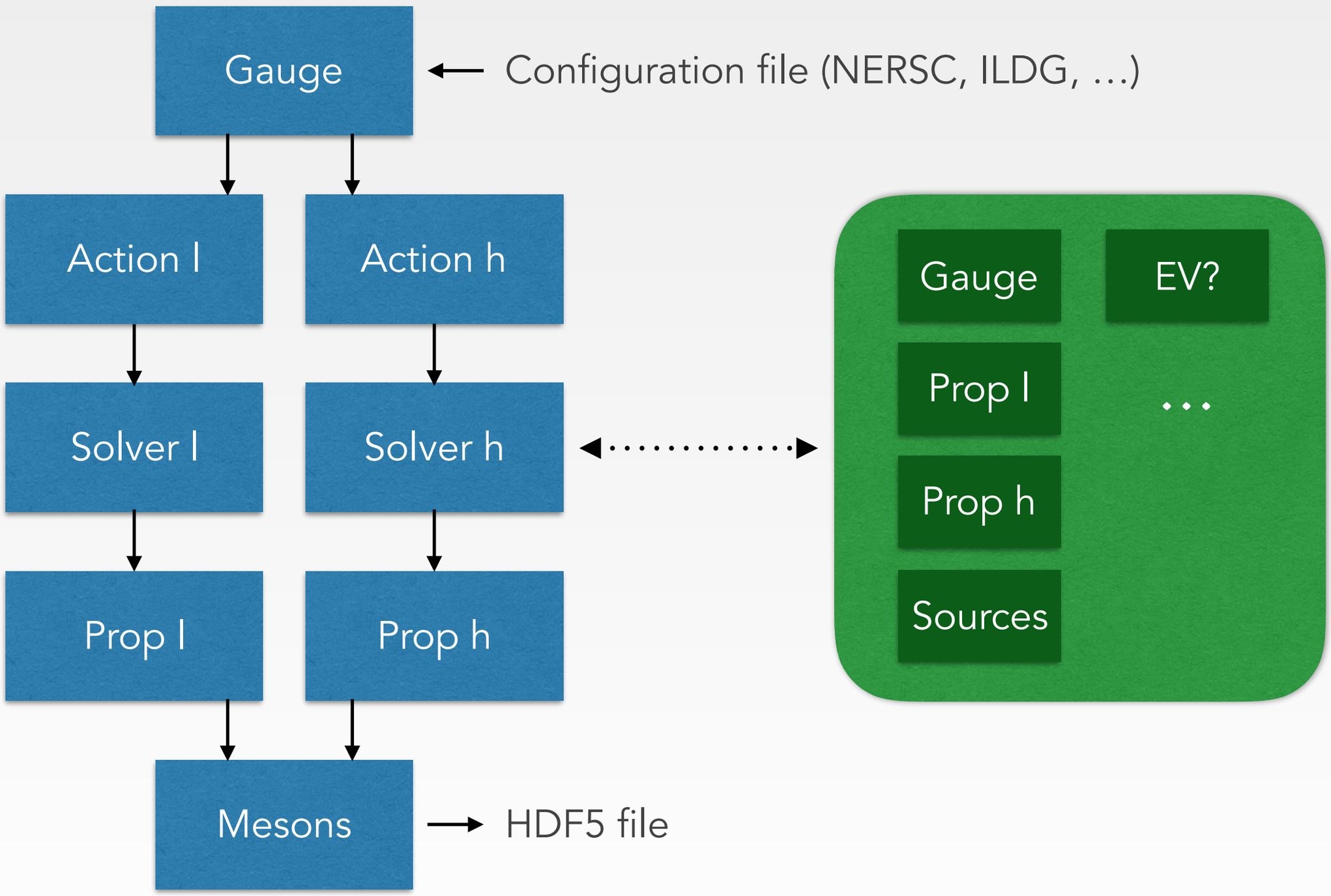
Directions for solutions

- **High modularity** — building a new project is easy.
- **Flexible I/O & control** — highly customisable input.
- **Automatic scheduling** — more self-consistency checks.

Measurement data flow



Measurement data flow



Scheduling

- Dataflow diagram: DAG.
- Dependency solving: DAG topological sort.
- Memory optimisation 1: garbage collection.
- Memory optimisation 2: constrained topological sort.
- Very likely NP-hard problem: need a heuristic solution.
- So far: genetic algorithm minimising high-water function on the space of topological sorts.
- Find a schedule in O(10 min) for big graphs, work in progress.

Productions workflows

- Heavy-light semi-leptonic decays using distillation
  O(1000) modules — Talk: Felix Erben
- Rare kaon decays
  O(1000) modules — Talk: Fionn Ó hÓgáin
- All-to-all IB corrections
  O(10) modules — Talk: James Richings
- IB corrections to light leptonic decays
  O(1000) modules — Talk: A.P.
- Holographic cosmology
  O(10) modules — Talk: Joseph Lee

Flexible control

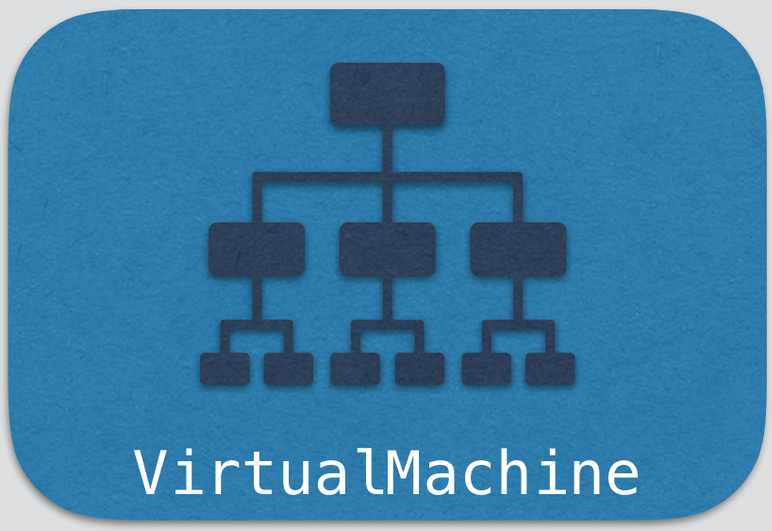
Hardcoded C++ ASCII input (*e.g.* XML)

- Hardcoded: risk of code (and bug) duplication.
- ASCII input: too general, complicated input.
- Matter of taste: user should be able to choose.
- Achieved with modules + Grid serialisable I/O.

Full structure

- Module DAG
- Scheduling & garbage collection

- Named object store
- Memory footprint aware



Application

High-level interface for VM setup

Hadrons::

```
using namespace Grid;
using namespace Hadrons;

int main(int argc, char *argv[])
{
    // initialization ////////////////////////////////////////////////////////
    Grid_init(&argc, &argv);
    HadronsLogError.Active(GridLogError.isActive());
    HadronsLogWarning.Active(GridLogWarning.isActive());
    HadronsLogMessage.Active(GridLogMessage.isActive());
    HadronsLogIterative.Active(GridLogIterative.isActive());
    HadronsLogDebug.Active(GridLogDebug.isActive());
    LOG(Message) << "Grid initialized" << std::endl;

    // run setup /////////////////////////////////////////////////////////////
    Application              application;
    std::vector<std::string> flavour = {"l", "s", "c1", "c2", "c3"};
    std::vector<double>      mass    = {.01, .04, .2  , .25 , .3  };

    // global parameters
    Application::GlobalPar globalPar;
    globalPar.trajCounter.start = 1500;
    globalPar.trajCounter.end   = 1520;
    globalPar.trajCounter.step  = 20;
    globalPar.seed              = "1 2 3 4";
    application.setPar(globalPar);

    // ... module enumeration

    // execution
    application.saveParameterFile("spectrum.xml");
    application.run();

    // epilogue
    LOG(Message) << "Grid is finalizing now" << std::endl;
    Grid_finalize();

    return EXIT_SUCCESS;
}
```

tests/hadrons/test_hadrons_spectrum.cc
(https://github.com/paboyle/Grid GPL v2)

```
// sources
MSource::Z2::Par z2Par;
z2Par.tA = 0;
z2Par.tB = 0;
application.createModule<MSource::Z2>("z2", z2Par);
MSource::Point::Par ptPar;
ptPar.position = "0 0 0 0";
application.createModule<MSource::Point>("pt", ptPar);
// sink
MSink::Point::Par sinkPar;
sinkPar.mom = "0 0 0";
application.createModule<MSink::ScalarPoint>("sink", sinkPar);

// set fermion boundary conditions to be periodic space, antiperiodic time.
std::string boundary = "1 1 1 -1";

for (unsigned int i = 0; i < flavour.size(); ++i)
{
    // actions
    MAction::DWF::Par actionPar;
    actionPar.gauge = "gauge";
    actionPar.Ls    = 12;
    actionPar.M5    = 1.8;
    actionPar.mass  = mass[i];
    actionPar.boundary = boundary;
    application.createModule<MAction::DWF>("DWF_" + flavour[i], actionPar);

    // solvers
    MSolver::RBPrecCG::Par solverPar;
    solverPar.action   = "DWF_" + flavour[i];
    solverPar.residual = 1.0e-8;
    application.createModule<MSolver::RBPrecCG>("CG_" + flavour[i],
                                                solverPar);

    // propagators
    MFermion::GaugeProp::Par quarkPar;
    quarkPar.solver = "CG_" + flavour[i];
    quarkPar.source = "pt";
    application.createModule<MFermion::GaugeProp>("Qpt_" + flavour[i], quarkPar);
    quarkPar.source = "z2";
    application.createModule<MFermion::GaugeProp>("QZ2_" + flavour[i], quarkPar);
}
```

`tests/hadrons/test_hadrons_spectrum.cc`
(https://github.com/paboyle/Grid GPL v2)

```cpp
// constructor ////////////////////////////////////////////////////////////////
template <typename FImpl>
TPoint<FImpl>::TPoint(const std::string name)
: Module<PointPar>(name)
{}

// dependencies/products //////////////////////////////////////////////////////
template <typename FImpl>
std::vector<std::string> TPoint<FImpl>::getInput(void)
{
    std::vector<std::string> in;

    return in;
}

template <typename FImpl>
std::vector<std::string> TPoint<FImpl>::getOutput(void)
{
    std::vector<std::string> out = {getName()};

    return out;
}

// setup //////////////////////////////////////////////////////////////////////
template <typename FImpl>
void TPoint<FImpl>::setup(void)
{
    envCreateLat(PropagatorField, getName());
}

// execution //////////////////////////////////////////////////////////////////
template <typename FImpl>
void TPoint<FImpl>::execute(void)
{
    LOG(Message) << "Creating point source at position [" << par().position
                 << "]" << std::endl;

    std::vector<int> position = strToVec<int>(par().position);
    auto             &src     = envGet(PropagatorField, getName());
    SitePropagator   id;

    id  = 1.;
    src = zero;
    pokeSite(id, src, position);
}
```

Hadrons/Modules/MSource/Point.hpp
(https://github.com/paboyle/Grid GPL v2)

Outlook

- Grid + Hadrons: cross-platform, high-performance lattice software.
- Grid: high-performance data parallel library.
- Hadrons: high-level interface focused on physics measurements.
- Modular structure, with automatic scheduling.
  Aimed at fast & future-proof project development.
- Already used in production for a wide variety of calculations.

Perspectives

- Still untested on GPUs, soon!
- More modules (Baryons, staggered, multi-grid, …).
- Scheduler optimisations.

Hadrons contributors

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