

How to measure residual mass and chiral condensate for the domain wall fermion using Hadrons code

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Hadrons Code

- The modified Hadrons code which can measure chiral condensate and two point meson correlator with source-sink separation lie in x direction, y direction, z direction and t direction is located in the following directory of Fugaku:

x dir: `/home/ra000001/a04428/src/modify_mres_finiteT/20220204_Add_Z2_psibarpsi_Hadrons.v20210716`

y dir: `/home/ra000001/a04428/src/modify_mres_finiteT/20220214_ydir_mres_Hadrons.v20210716`

z dir: `/home/ra000001/a04428/src/modify_mres_finiteT/20220214_zdir_mres_Hadrons.v20210716`

t dir: `/home/ra000001/a04428/src/20211216_Add_psibarpsi_Grid.v20210713`

How to create new module

- We need to create new modules for spatial meson correlator and chiral condensate, this can be done by executing the bash script `add_module_list.sh` in Hadrons code.

Determining the residual mass

- Residual chiral symmetry breaking of domain wall fermion due to finite L_s is characterized by residual mass m_{res}
- Measure the ratio of midpoint correlator to the pion correlator evaluated at large source-sink separations to remove the unphysical states contribution

$$m_{\text{res}} = R(t) = \frac{\left\langle \sum_{\vec{x}} J_{5q}^a(\vec{x}, t) \pi^a(\vec{0}, 0) \right\rangle}{\left\langle \sum_{\vec{x}} J_5^a(\vec{x}, t) \pi^a(\vec{0}, 0) \right\rangle}$$

Determining the residual mass

- $$m_{\text{res}} = R(t) = \frac{\sum_{\vec{x}} \left\langle J_{5q}^a(\vec{x}, t) \pi^a(\vec{0}, 0) \right\rangle}{\sum_{\vec{x}} \left\langle J_5^a(\vec{x}, t) \pi^a(\vec{0}, 0) \right\rangle}$$

Physical four dimensional fermion:

$$q(x) = P_L \Psi(x, 0) + P_R \Psi(x, L_s - 1); \quad \bar{q}(x) = \bar{\Psi}(x, L_s - 1) P_L + \bar{\Psi}(x, 0) P_R; \quad P_{L,R} = \frac{1 \pm \gamma_5}{2}$$

- $J_{5q}^a \approx m_{\text{res}} J_5^a$
- $J_5^a(x) = -\bar{\Psi}(x, L_s - 1) P_L t^a \Psi(x, 0) + \bar{\Psi}(x, 0) P_R t^a \Psi(x, L_s - 1) = \bar{q}(x) t^a \gamma_5 q(x)$
- $\pi^a(x) = i \bar{q}(x) t^a \gamma_5 q(x) = i J_5^a$

Motivation

$T = \frac{1}{aN_t}, N_t$ is rather short for finite T.

In this case, one usually determine the residual mass m_{res} by computing the ratio of the midpoint correlator to the pion correlator evaluated at source-sink separations which lie in a spatial rather than temporal direction.

Currently, Hadrons code has program for calculating the temporal meson correlator, but don't have program for spatial meson correlator.

How can we build spatial meson correlator program based on temporal meson correlator program ?

Temporal meson correlator

```
27 #include <Hadrons/Application.hpp>
28 #include <Hadrons/Modules.hpp>
29
30 using namespace Grid;
31 using namespace Hadrons;
32
33 int main(int argc, char *argv[])
34 {
35     // initialization //////////////////////////////////////
36     Grid_init(&argc, &argv);
37     HadronsLogError.Active(GridLogError.isActive());
38     HadronsLogWarning.Active(GridLogWarning.isActive());
39     HadronsLogMessage.Active(GridLogMessage.isActive());
40     HadronsLogIterative.Active(GridLogIterative.isActive());
41     HadronsLogDebug.Active(GridLogDebug.isActive());
42     LOG(Message) << "Grid initialized" << std::endl;
43
44     // run setup //////////////////////////////////////
45     Application application;
46     std::vector<std::string> flavour = {"l", "s", "c1", "c2", "c3"};
47     std::vector<double> mass = {.01, .04, .2, .25, .3};
48     unsigned int nt = GridDefaultLatt(1T);
49
50     // global parameters
51     Application::GlobalPar globalPar;
52     globalPar.trajCounter.start = 1500;
53     globalPar.trajCounter.end = 1520;
54     globalPar.trajCounter.step = 20;
55     globalPar.runId = "test";
56     globalPar.genetic.maxGen = 1000;
57     globalPar.genetic.maxCstGen = 200;
58     globalPar.genetic.popSize = 20;
59     globalPar.genetic.mutationRate = .1;
60     application.setPar(globalPar);
61
```

- Trajectory variables can be used to loop over configurations

Temporal meson correlator

```
62 // gauge field
63 application.createModule<MGauge::Unit>("gauge");
64
65 // set fermion boundary conditions to be periodic space, antiperiodic time.
66 std::string boundary = "1 1 1 -1";
67 std::string twist = "0. 0. 0. 0.";
68
69 // sink
70 MSink::Point::Par sinkPar;
71 sinkPar.mom = "0 0 0";
72 application.createModule<MSink::ScalarPoint>("sink", sinkPar);
73 for (unsigned int i = 0; i < flavour.size(); ++i)
74 {
75     // actions
76     MAction::DWF::Par actionPar;
77     actionPar.gauge = "gauge";
78     actionPar.Ls = 12;
79     actionPar.M5 = 1.8;
80     actionPar.mass = mass[i];
81     actionPar.boundary = boundary;
82     actionPar.twist = twist;
83     application.createModule<MAction::DWF>("DWF_" + flavour[i], actionPar);
84
85     // solvers
86     MSolver::RBPrecCG::Par solverPar;
87     solverPar.action = "DWF_" + flavour[i];
88     solverPar.residual = 1.0e-8;
89     solverPar.maxIteration = 10000;
90     application.createModule<MSolver::RBPrecCG>("CG_" + flavour[i],
91 solverPar);
92 }
```

Set all the link variables to one, so this program calculates correlators for the free case, if one wants to load nersc format configuration, use `MIO::LoadNersc`

Create a sink module "sink" at $p_x, p_y, p_z = 0$, the value of sink corresponds to $\vec{p} = 0$

Loop over all declared quarks to set for each flavor action, solver.

As action here it use domain wall fermion, where the gauge fields are from "gauge" and set $L_s=12$, $M_5=1.8$, mass corresponding to the flavor, boundary and twist are set. In line 83, it create a DWF action for the given flavor and name it "DWF_" + flavour[i]

To calculate the quark propagator, it needs to set a solver module which is used by propagator module. It use the module `MSolver::RBPrecCG`, where the action is given by the previous declared one, the residual and maximal iteration steps are set

RBPrecCG is a solver, it uses red black preconditioning and conjugate gradient method to obtain the propagator

Temporal meson correlator

```
93 for (unsigned int t = 0; t < nt; t += 1)
94
95     std::string srcName;
96     std::vector<std::string> qName;
97     std::vector<std::vector<std::string>> seqName;
98     // Z2 source
99     MSource::Z2::Par z2Par;
100    z2Par.tA = t;
101    z2Par.tB = t;
102    srcName = "z2_" + std::to_string(t);
103    application.createModule<MSource::Z2>(srcName, z2Par);
104    for (unsigned int i = 0; i < flavour.size(); ++i)
105    {
106        // sequential sources
107        MSource::SeqGamma::Par seqPar;
108        qName.push_back("QZ2_" + flavour[i] + "_" + std::to_string(t));
109        seqPar.q = qName[i];
110        seqPar.tA = (t + nt/4) % nt;
111        seqPar.tB = (t + nt/4) % nt;
112        seqPar.mom = "1. 0. 0. 0.";
113        seqName.push_back(std::vector<std::string>(Nd));
114        for (unsigned int mu = 0; mu < Nd; ++mu)
115        {
116            seqPar.gamma = 0x1 << mu;
117            seqName[i][mu] = "G" + std::to_string(seqPar.gamma)
118                + "_" + std::to_string(seqPar.tA) +
119                + qName[i];
120            application.createModule<MSource::SeqGamma>(seqName[i][mu], seqPar);
121        }
122        // propagators
123        MFermion::GaugeProp::Par quarkPar;
124        quarkPar.solver = "CG_" + flavour[i];
125        quarkPar.source = srcName;
126        application.createModule<MFermion::GaugeProp>(qName[i], quarkPar);
127        for (unsigned int mu = 0; mu < Nd; ++mu)
128        {
129            quarkPar.source = seqName[i][mu];
130            seqName[i][mu] = "Q_" + flavour[i] + "-" + seqName[i][mu];
131            application.createModule<MFermion::GaugeProp>(seqName[i][mu], quarkPar);
132        }
133    }
```


Temporal meson correlator

```

137 // contractions
138 MContraction::Meson::Par mesPar;
139 for (unsigned int i = 0; i < flavour.size(); ++i)
140 for (unsigned int j = i; j < flavour.size(); ++j)
141 {
142     mesPar.output = "mesons/Z2_" + flavour[i] + flavour[j];
143     mesPar.q1     = qName[i];
144     mesPar.q2     = qName[j];
145     mesPar.gammas = "all";
146     mesPar.sink   = "sink";
147     application.createModule<MContraction::Meson>("meson_Z2_"
148     + std::to_string(i)
149     + flavour[i]
150     + flavour[j],
151     mesPar);
152 }
153

```

```

181 // execution
182 application.saveParameterFile("meson2pt.xml");
183 application.run();
184
185 // epilogue
186 LOG(Message) << "Grid is finalizing now" << std::endl;
187 Grid_finalize();
188
189 return EXIT_SUCCESS;
190 }

```

$$\langle O_M(n) \bar{O}_M(l) \rangle_{DW} = -\text{tr} \left[\Gamma_A \left(\tilde{D}_{tov}^{-1}(m_{f_2}) \right)_{n,l} \Gamma_B \left(\tilde{D}_{tov}^{-1\dagger}(m_{f_1}) \right)_{n,l} \right]$$

Γ_A and Γ_B combination is set by the string parameter `mesPar.gammas`. For example if one wants to compute the correlator for $(\Gamma_A, \Gamma_B) = (\gamma_5, \gamma_y)$ and $(\Gamma_A, \Gamma_B) = (\gamma_x, 1)$

One would write:

`mesPar.gammas = " (Gamma5 GammaY) (GammaX Identity) "`

"all" option in line145 means compute the correlator for all 256 combinations of gamma matrices

After set all modules, store all the parameters in `"meson2pt.xml"`
 Start the execution with `application.run()`
 Use `Grid_finalize()` to destroy all created objects and free memory

Quark propagator

$$P_{L,R} = \frac{1 \pm \gamma_5}{2}$$

Physical four dimensional fermion:

$$q(x) = P_L \Psi(x,0) + P_R \Psi(x, L_s - 1); \quad \bar{q}(x) = \bar{\Psi}(x, L_s - 1) P_L + \bar{\Psi}(x,0) P_R$$

Physical propagator:

$$\langle \bar{q}(n) q(l) \rangle_{DW} = \frac{1}{Z_{DW}} \int \mathcal{D}\bar{\Psi} \mathcal{D}\Psi \mathcal{D}\bar{\Phi} \mathcal{D}\Phi \bar{q}(n) q(l) e^{-\bar{\Psi} D_{DW}(m) \Psi - \bar{\Phi} D_{DW}(1) \Phi}$$

$$= \frac{1}{1-m} \left([D_{tov}^{-1}(m)]_{l,n} - 1 \right) = [\tilde{D}_{tov}^{-1}(m)]_{l,n}$$

$$D_{tov}(m) = \frac{1+m}{2} + \frac{1-m}{2} \gamma_5 \epsilon_{L_s}(H), \quad \epsilon_{L_s}(H) = \frac{(1+H)^{L_s} - (1-H)^{L_s}}{(1+H)^{L_s} + (1-H)^{L_s}}, \quad \lim_{L_s \rightarrow \infty} D_{tov} = D_{ov}$$

$$H = \gamma_5 D_{kernel} = \gamma_5 \frac{(b_5 + c_5) D_W(-M_5)}{2 + (b_5 - c_5) D_W(-M_5)}$$

D_{kernel} is Mobius domain wall kernel

Inversion of the Dirac operator

The connection to the DWF operator

$$[\tilde{D}_{tov}^{-1}(m)]_{n,l} = [\mathbb{P}^\dagger D_{DW}^{-1}(m)(-D_-)\mathbb{P}^\dagger]_{n,l;0,L_s-1}, \quad \mathcal{P} = \begin{pmatrix} P_L & P_R & 0 & \dots & 0 \\ 0 & P_L & P_R & \dots & 0 \\ & & \dots & & \\ 0 & 0 & \dots & P_L & P_R \\ P_R & 0 & \dots & 0 & P_L \end{pmatrix} \quad P_{L,R} = \frac{1 \pm \gamma_5}{2}$$

To determine the propagator, need to do the inversion of the Dirac operator, it is time consuming

Introduce source to just invert a part of the operator, e.g. point source $\psi_0 = \delta_{n,n_0} \delta_{\alpha,\alpha_0} \delta_{a,a_0}$

$$\begin{aligned} [\tilde{D}_{tov}^{-1}(m)]_{n,l} [\psi_0]_l &= [\mathbb{P}^\dagger D_{DW}^{-1}(m)(-D_-)\mathbb{P}^\dagger]_{n,l;0,L_s-1} [\psi_0]_l \\ &= [\mathbb{P}^\dagger D_{DW}^{-1}(m)]_{n,l;0,s} [(-D_-)\mathbb{P}^\dagger \psi_0]_{l;s,L_s-1} \end{aligned}$$

$$= [\mathbb{P}^\dagger D_{DW}^{-1}(m)]_{n,l;0,s} [\Psi_{DW,0}]_{l;s,L_s-1} \quad \rightarrow \text{Five dimensional point source}$$

Solve $G = D_{DW}^{-1}(m)\Psi_{DW,0}$ using conjugate gradient (CG)

Then, project G back to four dimensions by $\mathbb{P}^\dagger G$ to get $[\tilde{D}_{tov}^{-1}(m)]_{n,n_0}$

Red black/even-odd preconditioning

$$\left[\tilde{D}_{tov}^{-1}(m)\right]_{n,l} [\psi_0]_l = \left[\tilde{D}_{tov}^{-1}(m)\right]_{n,n_0} = \left[\mathbb{P}^\dagger D_{DW}^{-1}(m)\right]_{n,l;0,s} \left[\Psi_{DW,0}\right]_{l;s,L_s-1}$$

- **Only calculate one column of the truncated overlap operator, reduced the time**

$$G = D_{DW}^{-1}(m) \Psi_{DW,0}$$

- **Need to do the above inversion for 12 sources which is all combinations of Dirac and color indices**
- **To further reduce the computational time, introduce red black preconditioning method**

Assign for each space-time point of the four dimensional lattice a parity $p = \{r, b\}$ with

$$p = (x + y + z + t) \bmod 2, \quad 0 \rightarrow r, 1 \rightarrow b$$

$$D_{DW} = \begin{pmatrix} M_{ee} & M_{eo} \\ M_{oe} & M_{oo} \end{pmatrix}$$

Red black/even-odd preconditioning

Shur decomposition

$$D_{DW} = \begin{pmatrix} M_{ee} & M_{eo} \\ M_{oe} & M_{oo} \end{pmatrix} \\ = \begin{pmatrix} 1 & 0 \\ M_{oe}M_{ee}^{-1} & 1 \end{pmatrix} \begin{pmatrix} M_{ee} & 0 \\ 0 & D_{oo} \end{pmatrix} \begin{pmatrix} 1 & M_{ee}^{-1}M_{eo} \\ 0 & 1 \end{pmatrix} = LDU$$

$$D_{DW}\psi = \eta$$

$$DU\psi = L^{-1}\eta$$

$$\begin{pmatrix} M_{ee} & M_{eo} \\ 0 & D_{oo} \end{pmatrix} \begin{pmatrix} \psi_e \\ \psi_o \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ -M_{oe}M_{ee}^{-1} & 1 \end{pmatrix} \begin{pmatrix} \eta_e \\ \eta_o \end{pmatrix}$$

$$\begin{pmatrix} M_{ee}\psi_e + M_{eo}\psi_o \\ D_{oo}\psi_o \end{pmatrix} = \begin{pmatrix} \eta_e \\ \eta_o - M_{oe}M_{ee}^{-1}\eta_e \end{pmatrix} = \begin{pmatrix} \eta_e \\ \eta'_o \end{pmatrix} \quad \rightarrow \quad D_{oo}\psi_o = \eta'_o$$

Solve $D_{oo}^\dagger D_{oo} \psi_o = D_{oo}^\dagger \eta'_o$

Put ψ_o into $\psi_e = M_{ee}^{-1}(\eta_e - M_{eo}\psi_o)$ **to get ψ_e**

Temporal meson correlator

Hadrons/Modules/MFermion/GaugeProp.hpp

```
216 template <typename FImpl>
217 void TGaugeProp<FImpl>::execute(void)
218 {
219     LOG(Message) << "Computing quark propagator '" << getName() << "'"
220         << std::endl;
221
222     std::string propName = (Ls_ == 1) ? getName() : (getName() + "_5d");
223
224     if (envHasType(PropagatorField, par().source))
225     {
226         auto &prop = envGet(PropagatorField, propName);
227         auto &propPhysical = envGet(PropagatorField, getName());
228         auto &fullSrc = envGet(PropagatorField, par().source);
229
230         LOG(Message) << "Using source '" << par().source << "'" << std::endl;
231         solvePropagator(prop, propPhysical, fullSrc);
232     }
233     else
234     {
235         auto &prop = envGet(std::vector<PropagatorField>, propName);
236         auto &propPhysical = envGet(std::vector<PropagatorField>, getName());
237         auto &fullSrc = envGet(std::vector<PropagatorField>, par().source);
238
239         for (unsigned int i = 0; i < fullSrc.size(); ++i)
240         {
241             LOG(Message) << "Using element " << i << " of source vector '"
242                 << par().source << "'" << std::endl;
243             solvePropagator(prop[i], propPhysical[i], fullSrc[i]);
244         }
245     }
246 }
```

Using red black preconditioning and the conjugate gradient method to solve the propagator

Hadrons/Modules/MFermion/GaugeProp.hpp

```

157 // execution //////////////////////////////////////
158 template <typename FImpl>
159 void TGaugeProp<FImpl>::solvePropagator(PropagatorField &prop,
160                                         PropagatorField &propPhysical,
161                                         const PropagatorField &fullSrc)
162 {
163     auto & solver = envGet(Solver, par().solver);
164     auto & mat = solver.getFMat();
165
166     envGetTmp(FermionField, source);
167     envGetTmp(FermionField, sol);
168     envGetTmp(FermionField, tmp);
169     LOG(Message) << "Inverting using solver " << par().solver << "
170     << std::endl;
171     for (unsigned int s = 0; s < Ns; ++s)
172     for (unsigned int c = 0; c < FImpl::Dimension; ++c)
173     {
174         LOG(Message) << "Inversion for spin= " << s << " color= " << c
175         << std::endl;
176         // source conversion for 4D sources
177         LOG(Message) << "Import source" << std::endl;
178         if (!env().isObject5d(par().source))
179         {
180             if (Ls_ == 1)
181             {
182                 PropToFerm<FImpl>(source, fullSrc, s, c);
183             }
184             else
185             {
186                 PropToFerm<FImpl>(tmp, fullSrc, s, c);
187                 mat.ImportPhysicalFermionSource(tmp, source);
188             }
189         }

```

```

190 // source conversion for 5D sources
191 else
192 {
193     if (Ls_ != env().getObjectLs(par().source))
194     {
195         HADRONS_ERROR(Size, "Ls mismatch between quark action and source");
196     }
197     else
198     {
199         PropToFerm<FImpl>(source, fullSrc, s, c);
200     }
201 }
202 sol = Zero();
203 LOG(Message) << "Solve" << std::endl;
204 solver(sol, source);
205 LOG(Message) << "Export solution" << std::endl;
206 FermToProp<FImpl>(prop, sol, s, c);
207 // create 4D propagators from 5D one if necessary
208 if (Ls_ > 1)
209 {
210     mat.ExportPhysicalFermionSolution(sol, tmp);
211     FermToProp<FImpl>(propPhysical, tmp, s, c);
212 }
213 }
214 }

```

$$\langle \bar{q}(n)q(l) \rangle_{DW} = [\tilde{D}_{tov}^{-1}(m)]_{l,n}$$

$$[\tilde{D}_{tov}^{-1}(m)]_{n,l} [\psi_0]_l = [\tilde{D}_{tov}^{-1}(m)]_{n,n_0} = [\mathbb{P}^\dagger D_{DW}^{-1}(m)]_{n,l;0,s} [\Psi_{DW,0}]_{l;s,L_s-1}$$

Solve $G = D_{DW}^{-1}(m)\Psi_{DW,0}$ using CG

Then project G back to four dimensions by $\mathbb{P}^\dagger G$ to get $[\tilde{D}_{tov}^{-1}(m)]_{n,n_0}$

Grid/algorithms/iterative/SchurRedBlack.h

```
template<class Guesser>
void operator() (Matrix &_Matrix, const Field &in, Field &out, Guesser &guess){
```

```
    // FIXME CGdiagonalMee not implemented virtual function
```

```
    // FIXME use CBfactorise to control schur decomp
```

```
    GridBase *grid = _Matrix.RedBlackGrid();
```

```
    GridBase *fgrid = _Matrix.Grid();
```

```
    Field resid(fgrid);
```

```
    Field src_o(grid);
```

```
    Field src_e(grid);
```

```
    Field sol_o(grid);
```

```
    //////////////////////////////////////
    // RedBlack source
    //////////////////////////////////////
    RedBlackSource(_Matrix, in, src_e, src_o);
```

```
    //////////////////////////////////////
    // Construct the guess
    //////////////////////////////////////
```

```
    if(useSolnAsInitGuess) {
        pickCheckerboard(0dd, sol_o, out);
    } else {
        guess(src_o, sol_o);
    }
}
```

```
    Field guess_save(grid);
    guess_save = sol_o;
```

```
    //////////////////////////////////////
    // Call the red-black solver
    //////////////////////////////////////
    RedBlackSolve(_Matrix, src_o, sol_o);
```

```
    //////////////////////////////////////
    // Fionn A2A boolean behavioural control
    //////////////////////////////////////
```

```
    if (subGuess) sol_o = sol_o - guess_save;
```

```
    //////////////////////////////////////
    // RedBlack solution needs the even source
    //////////////////////////////////////
    RedBlackSolution(_Matrix, sol_o, src_e, out);
```

```
    // Verify the unprec residual
```

```
    if (! subGuess) {
        _Matrix.M(out, resid);
        resid = resid - in;
        RealD ns = norm2(in);
        RealD nr = norm2(resid);
```

```
        std::cout << GridLogMessage << "SchurRedBlackBase solver true unprec resid " << std::sqrt(nr/ns) << std::endl;
```

```
    } else {
        std::cout << GridLogMessage << "SchurRedBlackBase Guess subtracted after solve." << std::endl;
    }
}
```


Grid/algorithms/iterative/SchurRedBlack.h

```
virtual void RedBlackSource(Matrix & _Matrix, const Field &src, Field &src_e, Field &src_o)
{
    GridBase *grid = _Matrix.RedBlackGrid();
    GridBase *fgrid = _Matrix.Grid();

    Field tmp(grid);
    Field Mtmp(grid);

    pickCheckerboard(Even, src_e, src);
    pickCheckerboard(Odd, src_o, src);

    //////////////////////////////////////
    // src_o = Mdag * (source_o - Moe MeeInv source_e)
    //////////////////////////////////////

    _Matrix.MoeeeInv(src_e, tmp);      assert( tmp.Checkerboard() ==Even);
    _Matrix.Meooo (tmp, Mtmp);        assert( Mtmp.Checkerboard() ==Odd);
    tmp=src_o-Mtmp;                   assert( tmp.Checkerboard() ==Odd);

    // get the right MpcDag
    SchurDiagMoeeeOperator<Matrix, Field> _HermOpEO(_Matrix);
    _HermOpEO.MpcDag(tmp, src_o);    assert(src_o.Checkerboard() ==Odd);
}
}
```

$$\eta'_o = \eta_o - M_{oe}M_{ee}^{-1}\eta_e$$

$$D_{oo} = M_{oo} - M_{oe}M_{ee}^{-1}M_{eo}$$

$$D_{oo}^\dagger \eta'_o$$


```

120 SolverTimer.Start();
121 int k;
122 for (k = 1; k <= MaxIterations; k++) {
123     c = cp;
124
125     MatrixTimer.Start();
126     Linop.HermOp(p, mmp);
127     MatrixTimer.Stop();

```

$$out = -1 \times tmp + out = -1 \times (M_{oe} M_{ee}^{-1} M_{eo} P_{o(i)}) + M_{oo} P_{o(i)} = D_{oo} P_{o(i)}$$

$$mmp = D_{oo}^\dagger D_{oo} P_{o(i)}$$

```

233 virtual void HermOp(const Field &in, Field &out) {
234     out.Checkerboard() = in.Checkerboard();
235     MpcDagMpc(in, out);
236 }

```

```

259 virtual void Mpc (const Field &in, Field &out) {
260     Field tmp(in.Grid());
261     tmp.Checkerboard() = !in.Checkerboard();
262
263     _Mat.Meooe(in, tmp);
264     _Mat.MooeeInv(tmp, out);
265     _Mat.Meooe(out, tmp);
266     _Mat.Mooee(in, out);
267     axpy(out, -1.0, tmp, out);
268 }
269 virtual void MpcDag (const Field &in, Field &out) {
270     Field tmp(in.Grid());
271
272     _Mat.MeooeDag(in, tmp);
273     _Mat.MooeeInvDag(tmp, out);
274     _Mat.MeooeDag(out, tmp);
275     _Mat.MooeeDag(in, out);
276     axpy(out, -1.0, tmp, out);
277 }

```

$$out = D_{oo}^\dagger D_{oo} P_{o(i)}$$

```

220 virtual void MpcDagMpc(const Field &in, Field &out) {
221     Field tmp(in.Grid());
222     tmp.Checkerboard() = in.Checkerboard();
223     Mpc(in, tmp);
224     MpcDag(tmp, out);
225 }

```

Grid/algorithms/iterative/SchurRedBlack.h

$$D_{oo} = M_{oo} - M_{oe}M_{ee}^{-1}M_{eo}$$

```
virtual void RedBlackSolve (Matrix & _Matrix, const Field &src_o, Field &sol_o)
{
  SchurDiagMoeeeOperator<Matrix,Field> _HermOpE0(_Matrix);
  this->_HermitianRBSolver(_HermOpE0,src_o,sol_o); assert(sol_o.Checkerboard()==0dd);
};
```

$$\text{src_o} = D_{oo}^\dagger \eta'_o$$

$$\text{sol_o} = \psi_o$$

$$\text{CG: } D_{oo}^\dagger D_{oo} \psi_o = D_{oo}^\dagger \eta'_o$$

Grid/algorithms/iterative/ConjugateGradient.h

CG:

```
59 void operator()(LinearOperatorBase<Field> &Linop, const Field &src, Field &psi) {
60     psi.Checkerboard() = src.Checkerboard();
61     conformable(psi, src);
62     RealD cp, c, a, d, b, ssq, qq;
63     //RealD b_pred;
64     Field p(src);
65     Field mmp(src);
66     Field r(src);
67
68     // Initial residual computation & set up
69     RealD guess = norm2(psi);
70     assert(std::isnan(guess) == 0);
71     Linop.HermOpAndNorm(psi, mmp, d, b);
72
73     r = src - mmp;
74     p = r;
75
76     a = norm2(p);
77     cp = a;
78     ssq = norm2(src);
79
80     // Handle trivial case of zero src
81     if (ssq == 0.){
82         psi = Zero();
83         IterationsToComplete = 1;
84         TrueResidual = 0.;
85         return;
86     }
87
88     std::cout << GridLogIterative << std::setprecision(8) << "ConjugateGradient: guess "
89     << guess << std::endl;
```

$$r(0) = b - Ax(0)$$

$$p(0) = r(0)$$

$$r(i)^\dagger r(i)$$

```
94     std::cout << GridLogIterative << std::setprecision(8) << "ConjugateGradient: src "
95     << ssq << std::endl;
96     std::cout << GridLogIterative << std::setprecision(8) << "ConjugateGradient: mp "
97     << d << std::endl;
98     std::cout << GridLogIterative << std::setprecision(8) << "ConjugateGradient: mmp "
99     << b << std::endl;
100    std::cout << GridLogIterative << std::setprecision(8) << "ConjugateGradient: cp,r "
101    << cp << std::endl;
102    std::cout << GridLogIterative << std::setprecision(8) << "ConjugateGradient: p "
103    << a << std::endl;
104
105    RealD rsq = Tolerance * Tolerance * ssq;
106
107    // Check if guess is really REALLY good
108    if (cp <= rsq) {
109        TrueResidual = std::sqrt(a/ssq);
110        std::cout << GridLogMessage << "ConjugateGradient guess is converged already " << s
111        << std::endl;
112        IterationsToComplete = 0;
113        return;
114    }
115
116    std::cout << GridLogIterative << std::setprecision(8)
117    << "ConjugateGradient: k=0 residual: cp << " target " << rsq << std::en
118    dl;
119
120    GridStopWatch LinalgTimer;
121    GridStopWatch InnerTimer;
122    GridStopWatch AxdyNormTimer;
123    GridStopWatch LinearCombTimer;
124    GridStopWatch MatrixTimer;
125    GridStopWatch SolverTimer;
```



```

120 SolverTimer.Start();
121 int k;
122 for (k = 1; k <= MaxIterations; k++) {
123     c = cp;
124     MatrixTimer.Start();
125     Linop.HermOp(p, mmp);
126     MatrixTimer.Stop();
127     LinalgTimer.Start();
128     InnerTimer.Start();
129     ComplexD dc = innerProduct(p, mmp);
130     InnerTimer.Stop();
131     d = dc.real();
132     a = c / d;
133     AxyNormTimer.Start();
134     cp = axpy_norm(r, -a, mmp, r);
135     AxyNormTimer.Stop();
136     b = cp / c;
137     LinearCombTimer.Start();
138     {
139     autoView( psi_v , psi, AcceleratorWrite);
140     autoView( p_v   , p,   AcceleratorWrite);
141     autoView( r_v   , r,   AcceleratorWrite);
142     accelerator_for(ss, p_v.size(), Field::vector_object::Nsimd(), {
143     coalescedWrite(psi_v[ss], a * p_v(ss) + psi_v(ss));
144     coalescedWrite(p_v[ss] , b * p_v(ss) + r_v (ss));
145     });
146     LinearCombTimer.Stop();
147     LinalgTimer.Stop();
148     std::cout << GridLogIterative << "ConjugateGradient: Iteration " << k
149     << " residual " << sqrt(cp/ssq) << " target " << Tolerance << std::endl;
150 }
151 }
152 }
153 }
154 }
155 }
156 }
157 }

```

$$r_{(i)}^\dagger r_{(i)}$$

$$Ap_{(i)}$$

$$p_{(i)}^\dagger Ap_{(i)}$$

$$\alpha_{(i)} = \frac{r_{(i)}^\dagger r_{(i)}}{p_{(i)}^\dagger Ap_{(i)}}$$

$$r_{(i+1)} = r_{(i)} - \alpha_{(i)} Ap_{(i)}$$

$$r_{(i+1)}^\dagger r_{(i+1)}$$

$$\beta_{(i+1)} = \frac{r_{(i+1)}^\dagger r_{(i+1)}}{r_{(i)}^\dagger r_{(i)}}$$

$$x_{(i+1)} = x_{(i)} + \alpha_{(i)} p_{(i)},$$

$$p_{(i+1)} = r_{(i+1)} + \beta_{(i+1)} p_{(i)},$$

Grid/algorithms/iterative/ConjugateGradient.h

```
158 // Stopping condition
159 if (cp <= rsq) {
160     SolverTimer.Stop();
161     Linop.HermOpAndNorm(psi, mmp, d, qq);
162     p = mmp - src;
163
164     RealD srcnorm = std::sqrt(norm2(src));
165     RealD resnorm = std::sqrt(norm2(p));
166     RealD true_residual = resnorm / srcnorm;
167
168     std::cout << GridLogMessage << "ConjugateGradient Converged on iteration " << k
169     << "\tComputed residual " << std::sqrt(cp / ssq)
170     << "\tTrue residual " << true_residual
171     << "\tTarget " << Tolerance << std::endl;
172
173     std::cout << GridLogIterative << "Time breakdown " << std::endl;
174     std::cout << GridLogIterative << "\tElapsed " << SolverTimer.Elapsed() << std::endl;
175     std::cout << GridLogIterative << "\tMatrix " << MatrixTimer.Elapsed() << std::endl;
176     std::cout << GridLogIterative << "\tLinalg " << LinalgTimer.Elapsed() << std::endl;
177     std::cout << GridLogIterative << "\tInner " << InnerTimer.Elapsed() << std::endl;
178     std::cout << GridLogIterative << "\tAxyNorm " << AxyNormTimer.Elapsed() << std::endl;
179     std::cout << GridLogIterative << "\tLinearComb " << LinearCombTimer.Elapsed() << std::endl;
180
181     if (ErrorOnNoConverge) assert(true_residual / Tolerance < 10000.0);
182
183     IterationsToComplete = k;
184     TrueResidual = true_residual;
185
186     return;
187 }
188 }
189 // Failed. Calculate true residual before giving up
190 Linop.HermOpAndNorm(psi, mmp, d, qq);
191 p = mmp - src;
192
193 TrueResidual = sqrt(norm2(p)/ssq);
194
195 std::cout << GridLogMessage << "ConjugateGradient did NOT converge " << k << " / " << MaxIterations << std::endl;
196
197 if (ErrorOnNoConverge) assert(0);
198 IterationsToComplete = k;
199
200 }
```


Grid/algorithms/iterative/SchurRedBlack.h

```

virtual void RedBlackSolution(Matrix& _Matrix, const Field& sol_o, const Field& src_e, Field& sol)
{
    GridBase* grid = _Matrix.RedBlackGrid();
    GridBase* fgrid = _Matrix.Grid();

    Field tmp(grid);
    Field sol_e(grid);
    Field src_e_i(grid);

    ////////////////////////////////////////
    // sol_e = M_ee^-1 * ( src_e - Meo sol_o )...
    ////////////////////////////////////////
    _Matrix.Meooe(sol_o, tmp);      assert( tmp.Checkerboard() == Even );
    src_e_i = src_e - tmp;         assert( src_e_i.Checkerboard() == Even );
    _Matrix.MooeeInv(src_e_i, sol_e); assert( sol_e.Checkerboard() == Even );

    setCheckerboard(sol, sol_e); assert( sol_e.Checkerboard() == Even );
    setCheckerboard(sol, sol_o); assert( sol_o.Checkerboard() == Odd );
}

```

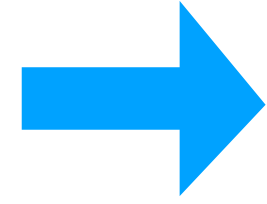
$$\psi_e = M_{ee}^{-1} (\eta_e - M_{eo} \psi_o)$$

Solve $D_{oo}^\dagger D_{oo} \psi_o = D_{oo}^\dagger \eta'_o$

Put ψ_o into $\psi_e = M_{ee}^{-1} (\eta_e - M_{eo} \psi_o)$ to get ψ_e

Temporal meson correlator

$$\langle O_M(n) \bar{O}_M(l) \rangle_{DW} = \left\langle \bar{q}^{f_1(n)\alpha_1} \Gamma_{\alpha_1\beta_1} q^{f_2(n)\beta_1} \bar{q}^{f_2(l)\alpha_2} \Gamma_{\alpha_2\beta_2} q^{f_1(l)\beta_2} \right\rangle_{DW} = -\Gamma_{\alpha_1\beta_1} \Gamma_{\alpha_2\beta_2} \left\langle \bar{q}^{f_2(l)\alpha_2} q^{f_2(n)\beta_1} \right\rangle_{DW} \left\langle \bar{q}^{f_1(n)\alpha_1} q^{f_1(l)\beta_2} \right\rangle_{DW}$$

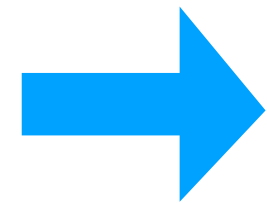


Fermion contraction

$$= -\Gamma_{\alpha_1\beta_1} \Gamma_{\alpha_2\beta_2} \frac{1}{1-m_{f_2}} \left(\left[D_{tov}^{-1}(m_{f_2}) \right]_{n,l} - 1 \right)_{\substack{\beta_1\alpha_2 \\ a_1a_2}} \frac{1}{1-m_{f_1}} \left(\left[D_{tov}^{-1}(m_{f_1}) \right]_{l,n} - 1 \right)_{\substack{\beta_2\alpha_1 \\ a_2a_1}}$$

$$= -\text{tr} \left[\Gamma \left(\tilde{D}_{tov}^{-1}(m_{f_2}) \right)_{n,l} \Gamma \left(\tilde{D}_{tov}^{-1}(m_{f_1}) \right)_{l,n} \right] \quad \text{where} \quad \left(\tilde{D}_{tov}^{-1}(m_{f_i}) \right)_{n,l} = \frac{1}{1-m_{f_i}} \left(\left[D_{tov}^{-1}(m_{f_i}) \right]_{n,l} - 1 \right)$$

Trace is over spin and color index



γ_5 **hermiticity** : $\left[\tilde{D}_{tov}^{-1}(m) \right]_{l,n} = \gamma_5 \left[\tilde{D}_{tov}^{-1\dagger}(m) \right]_{n,l} \gamma_5$

$$\langle O_M(n) \bar{O}_M(l) \rangle_{DW} = -\text{tr} \left[(\gamma_5 \Gamma) \left(\tilde{D}_{tov}^{-1}(m_{f_2}) \right)_{n,l} (\Gamma \gamma_5) \left(\tilde{D}_{tov}^{-1\dagger}(m_{f_1}) \right)_{n,l} \right]$$

Only need to calculate the propagator of one direction

Two point meson correlator at zero momentum:

$$C(t) = \sum_{\vec{x}} \langle O_M(\vec{x}, t) \bar{O}_M(0,0) \rangle$$

Temporal meson correlator

Hadrons/Modules/MContraction/Meson.hpp

```
// execution //////////////////////////////////////
#define mesonConnected(q1, q2, gSnk, gSrc) \
(g5*(gSnk))*(q1)*(adj(gSrc)*g5)*adj(q2)
template <typename FImpl1, typename FImpl2>
void TMeson<FImpl1, FImpl2>::execute(void)
{
    LOG(Message) << "Computing meson contractions " << getName() << " using "
    << " quarks " << par().q1 << " and " << par().q2 << " "
    << std::endl;

    std::vector<TComplex> buf;
    std::vector<Result> result;
    Gamma g5(Gamma::Algebra::Gamma5);
    std::vector<GammaPair> gammaList;
    int nt = env().getDim(Tp);

    parseGammaString(gammaList);
    result.resize(gammaList.size());
    for (unsigned int i = 0; i < result.size(); ++i)
    {
        result[i].gamma_snk = gammaList[i].first;
        result[i].gamma_src = gammaList[i].second;
        result[i].corr.resize(nt);
    }
}
```

```
auto &q1 = envGet(PropagatorField1, par().q1);
auto &q2 = envGet(PropagatorField2, par().q2);

envGetTmp(LatticeComplex, c);
LOG(Message) << "(using sink " << par().sink << ")" << std::endl;
for (unsigned int i = 0; i < result.size(); ++i)
{
    Gamma gSnk(gammaList[i].first);
    Gamma gSrc(gammaList[i].second);
    std::string ns;

    ns = vm().getModuleNamespace(env().getObjectModule(par().sink));
    if (ns == "MSource")
    {
        PropagatorField1 &sink = envGet(PropagatorField1, par().sink);
        c = trace(mesonConnected(q1, q2, gSnk, gSrc)*sink);
        sliceSum(c, buf, Tp);
    }
    else if (ns == "MSink")
    {
        SinkFnScalar &sink = envGet(SinkFnScalar, par().sink);
        c = trace(mesonConnected(q1, q2, gSnk, gSrc));
        buf = sink(c);
    }
    for (unsigned int t = 0; t < buf.size(); ++t)
    {
        result[i].corr[t] = TensorRemove(buf[t]);
    }
}

saveResult(par().output, "meson", result);
```

Tp denotes the lattice temporal direction, its value is 3, nt is maximal extension of temporal direction.

q₁, q₂ are quark propagators
 gSnk, gSrc ∈ Γ_i (i = 0, 1, ...15)
 t = 0, 1, ...N_t - 1

$$\text{tr} \left[\gamma_5 \Gamma_{\text{snk}} q_1 (\Gamma_{\text{src}} \gamma_5)^\dagger q_2^\dagger \right]$$

Temporal meson correlator

```
else if (ns == "MSink")
{
    SinkFnScalar &sink = envGet(SinkFnScalar, par().sink);

    c = trace(mesonConnected(q1, q2, gSnk, gSrc));
    buf = sink(c);
}
for (unsigned int t = 0; t < buf.size(); ++t)
{
    result[i].corr[t] = TensorRemove(buf[t]);
}
}
saveResult(par().output, "meson", result);
```

$$C(t) = \sum_{x,y,z} \text{tr} \left[\gamma_5 \Gamma_{\text{snk}} q_1 (\Gamma_{\text{src}} \gamma_5)^\dagger q_2^\dagger \right]$$

```
// execution //////////////////////////////////////
////
template <typename FImpl>
void TSourceSink<FImpl>::execute(void)
{
    LOG(Message) << "Setting up sink function with source '" << par().source
e << "' as the sink" << std::endl;

    PropagatorField &source = envGet(PropagatorField, par().source);

    auto sink = [this, source](const PropagatorField &field)
    {
        SlicedPropagator res;
        PropagatorField tmp = source*field;
        sliceSum(tmp, res, Tp);

        return res;
    };
    envGet(SinkFn, getName()) = sink;
}
```

sliceSum function summing over all lattice sites in slices orthogonal to the Tp direction. Tp is 3, represent the temporal direction.

Temporal meson correlator -> Spatial meson correlator

```

178 template <typename FImpl1, typename FImpl2>
179 void TMeson<FImpl1, FImpl2>::execute(void)
180 {
181     LOG(Message) << "Computing meson contractions " << getName() << " using "
182         << " quarks " << par().q1 << " and " << par().q2 << " in "
183         << std::endl;
184
185     std::vector<TComplex> buf;
186     std::vector<Result> result;
187     Gamma g5(Gamma::Algebra::Gamma5);
188     std::vector<GammaPair> gammaList;
189     int nt = env().getDim(Tp);
190

```

```

else if (ns == "MSink")
{
    SinkFnScalar &sink = envGet(SinkFnScalar, par().sink);
    c = trace(mesonConnected(q1, q2, gSnk, gSrc));
    buf = sink(c);
}
for (unsigned int t = 0; t < buf.size(); ++t)
{
    result[i].corr[t] = TensorRemove(buf[t]);
}
}
saveResult(par().output, "meson", result);

```

```

// execution //////////////////////////////////////
////
template <typename FImpl>
void TSourceSink<FImpl>::execute(void)
{
    LOG(Message) << "Setting up sink function with source " << par().source
    e << " as the sink" << std::endl;
    PropagatorField &source = envGet(PropagatorField, par().source);
    auto sink = [this, source](const PropagatorField &field)
    {
        SlicedPropagator res;
        PropagatorField tmp = source*field;
        sliceSum(tmp, res, Tp);
        return res;
    };
    envGet(SinkFn, getName()) = sink;
}

```

To get meson correlator in spatial direction:

$$\text{e.g. } C(x) = \sum_{y,z,t} \text{tr} \left[\gamma_5 \Gamma_{\text{snk}} q_1 (\Gamma_{\text{src}} \gamma_5)^\dagger q_2^\dagger \right]$$

Change Tp of these two parts into Xp

Xp, Yp, Zp, Tp are global integer variables of Grid and also of Hadrons, which denote the lattice directions
Its corresponding values are 0,1,2,3


```

160 // execution //////////////////////////////////////
161 template <typename FImpl>
162 void TWardIdentity<FImpl>::execute(void)
163 {
164     LOG(Message) << "Performing Ward Identity checks for propagator " << par().prop << std::endl;
165     auto &prop = envGet(PropagatorField, par().prop);
166     LOG(Message) << "Action " << par().action << std::endl;
167     auto &act = envGet(FMat, par().action);
168     LOG(Message) << "Physical source " << par().source << std::endl;
169     auto &phys_source = envGet(PropagatorField, par().source);
170     Gamma g5(Gamma::Algebra::Gamma5);
171     Gamma gT(Gamma::Algebra::GammaT);
172
173     // Create results = zero
174     Result result;
175     result.mass = par().mass;
176     const int nx { env().getDim(X) };
177     result.DmuJmu.resize(nx, 0.);
178     result.VDmuJmu.resize(nx, 0.);
179     result.PJ5q.resize(nx, 0.);
180     result.PA0.resize(nx, 0.);
181
182     // Compute D_mu V_mu (D here is backward derivative)
183     // There is no point performing Dmu on spatial directions, because after the spatial sum, these become zero
184     envGetTmp(PropagatorField, tmp);
185     envGetTmp(ComplexField, tmp_current);
186     SlicedComplex sumSV(nx);

```

```

187     SlicedComplex sumVV(nx);
188     LOG(Message) << "Getting vector conserved current" << std::endl;
189     act.ContractConservedCurrent(prop, prop, tmp, phys_source, Current::Vector, Xdir);
190     // Scalar-vector current density
191     tmp_current = trace(tmp);
192     SliceOut(result.DmuJmu, sumSV, tmp_current, true);
193     // Vector-vector current density
194     tmp_current = trace(gT*tmp);
195     SliceOut(result.VDmuJmu, sumVV, tmp_current, true);

```



```

207 // Test axial Ward identity for 5D actions
208 if (Ls_ > 1)
209 {
210     LOG(Message) << "Getting axial conserved current" << std::endl;
211     act.ContractConservedCurrent(prop, prop, tmp, phys_source, Current::Axial, Xdir);
212     // Pseudoscalar-Axial current density
213     tmp_current = trace(g5 * tmp);
214     SlicedComplex sumPA(nx);
215     // Save temporal component of pseudoscalar-(partially) conserved axial
216     // \mathcal{A}_0 from eq (37) in https://arxiv.org/pdf/hep-lat/0612005.pdf
217     SliceOut(result.PA0, sumPA, tmp_current, false);
218     // <PJ5q>
219     act.ContractJ5q(prop, tmp_current);
220     SlicedComplex sumPJ5q(nx);
221     SliceOut(result.PJ5q, sumPJ5q, tmp_current, false);
222 }
223
224 LOG(Message) << "Writing results to " << par().output << "." << std::endl;
225 saveResult(par().output, "wardIdentity", result);
226 }

```



```

611 template <class Impl>
612 void CayleyFermion5D<Impl>::ContractJ5q(PropagatorField &q_in, ComplexField &J5q)
613 {
614     conformable(this->GaugeGrid(), J5q.Grid());
615     conformable(q_in.Grid(), this->FermionGrid());
616     Gamma G5(Gamma::Algebra::Gamma5);
617     // 4d field
618     int Ls = this->Ls;
619     PropagatorField psi(this->GaugeGrid());
620     PropagatorField p_plus(this->GaugeGrid());
621     PropagatorField p_minus(this->GaugeGrid());
622     PropagatorField p(this->GaugeGrid());
623
624     ExtractSlice(p_plus, q_in, Ls/2-1, 0);
625     ExtractSlice(p_minus, q_in, Ls/2, 0);
626     p_plus = p_plus + G5*p_plus;
627     p_minus = p_minus - G5*p_minus;
628     p = 0.5*(p_plus+p_minus);
629     J5q = localInnerProduct(p,p);
630 }

```

$$P_{\text{-plus}} = (1 + \gamma_5) \psi(x, \frac{L_s}{2} - 1), \quad P_{\text{-minus}} = (1 - \gamma_5) \psi(x, \frac{L_s}{2})$$

$$P = \frac{1}{2} \left[(1 + \gamma_5) \psi(x, \frac{L_s}{2} - 1) + (1 - \gamma_5) \psi(x, \frac{L_s}{2}) \right]$$

$$P_L = \frac{1 - \gamma_5}{2}, \quad P_R = \frac{1 + \gamma_5}{2}$$

$$J_{5q} = P^\dagger P = \bar{\psi}(x, \frac{L_s}{2} - 1) P_L \psi(x, \frac{L_s}{2}) + \bar{\psi}(x, \frac{L_s}{2}) P_R \psi(x, \frac{L_s}{2} - 1)$$

$$P = P_R \psi(x, \frac{L_s}{2} - 1) + P_L \psi(x, \frac{L_s}{2})$$

$$P^\dagger = \bar{\psi}(x, \frac{L_s}{2} - 1) P_L + \bar{\psi}(x, \frac{L_s}{2}) P_R$$

$$P_R P_L = P_L P_R = 0, \quad P_L^2 = P_L, \quad P_R^2 = P_R$$

./Grid/lattice/Lattice_transfer.h

```
656 template<class vobj>
657 void ExtractSlice(Lattice<vobj> &lowDim,const Lattice<vobj> & higherDim,int slice, int orthog)
658 {
659     typedef typename vobj::scalar_object sobj;
660
661     GridBase *lg = lowDim.Grid();
662     GridBase *hg = higherDim.Grid();
663     int nl = lg->_ndimension;
664     int nh = hg->_ndimension;
665
666     assert(nl+1 == nh);
667     assert(orthog<nh);
668     assert(orthog>=0);
669     assert(hg->_processors[orthog]==1);
670
671     int dl; dl = 0;
672     for(int d=0;d<nh;d++){
673         if ( d != orthog) {
674             assert(lg->_processors[d] == hg->_processors[d]);
675             assert(lg->_ldimensions[d] == hg->_ldimensions[d]);
676             dl++;
677         }
678     }
679     // the above should guarantee that the operations are local
680     autoView(lowDimv,lowDim,CpuWrite);
681     autoView(higherDimv,higherDim,CpuRead);
682     thread_for(idx,lg->lSites(),{
683         sobj s;
684         Coordinate lcoor(nl);
685         Coordinate hcoor(nh);
686         lg->LocalIndexToLocalCoor(idx,lcoor);
687         int ddl=0;
688         hcoor[orthog] = slice;
689         for(int d=0;d<nh;d++){
690             if ( d!=orthog ) {
691                 hcoor[d]=lcoor[ddl++];
692             }
693         }
694         peekLocalSite(s,higherDimv,hcoor);
695         pokeLocalSite(s,lowDimv,lcoor);
696     });
697
698 }
```

Slices between grid of dimension N
and grid of dimensions N+1


```

207 // Test axial Ward identity for 5D actions
208 if (Ls_ > 1)
209 {
210     LOG(Message) << "Getting axial conserved current" << std::endl;
211     act.ContractConservedCurrent(prop, prop, tmp, phys_source, Current::Axial, Xdir);
212     // Pseudoscalar-Axial current density
213     tmp_current = trace(g5 * tmp);
214     SlicedComplex sumPA(nx);
215     // Save temporal component of pseudoscalar-(partially) conserved axial
216     // \mathcal{A}_0 from eq (37) in https://arxiv.org/pdf/hep-lat/0612005.pdf
217     SliceOut(result.PA0, sumPA, tmp_current, false);
218     // <P|J5q>
219     act.ContractJ5q(prop, tmp_current);
220     SlicedComplex sumPJ5q(nx);
221     SliceOut(result.PJ5q, sumPJ5q, tmp_current, false);
222 }

```

```

101 // Perform Slice Sum and then save delta
102 void SliceOut(std::vector<Complex> &Out, SlicedComplex &Sum, const ComplexField &f, bool bDiff) const
103 {
104     sliceSum(f, Sum, Xp);
105     const auto nx = Sum.size();
106     for (size_t t = 0; t < nx; ++t)
107     {
108         Out[t] = TensorRemove(bDiff ? Sum[t] - Sum[(t-1+nx)%nx] : Sum[t]);
109     }
110 }

```

How to obtain the chiral condensate

$$D_{DWF}\psi = \eta$$


- After the solver, add function

```
auto result = innerProduct(src, sol)
```

$$\text{result} = \eta^\dagger \psi$$

How to obtain the chiral condensate

- We need to create a new module for chiral condensate using bash script `make_module_list.sh` in Hadrons code and then make some changes as mentioned in the previous slide

Backup

Output file:

```
84 Hadrons : Message : 1.207894 s : Schedule (memory needed: 527.0 MB):
85 Hadrons : Message : 1.207913 s : 1: sink
86 Hadrons : Message : 1.207926 s : 2: gauge
87 Hadrons : Message : 1.207933 s : 3: smgauge
88 Hadrons : Message : 1.207942 s : 4: DWF_l
89 Hadrons : Message : 1.207949 s : 5: CG_l
90 Hadrons : Message : 1.207957 s : 6: pt
91 Hadrons : Message : 1.207963 s : 7: Qpt_l
92 Hadrons : Message : 1.207969 s : 8: meson_pt_ll
93 Hadrons : Message : 1.207975 s : 9: WTI_pt_ll
94 Hadrons : Message : 1.207981 s : 10: walk
95 Hadrons : Message : 1.207987 s : 11: Qwalk_l
96 Hadrons : Message : 1.207993 s : 12: meson_walk_ll
97 Hadrons : Message : 1.207999 s : 13: WTI_walk_ll
98 Hadrons : Message : 1.208005 s : 14: Z2
99 Hadrons : Message : 1.208011 s : 15: QZ2_l
100 Hadrons : Message : 1.208017 s : 16: meson_Z2_ll
101 Hadrons : Message : 1.208023 s : 17: WTI_Z2_ll
```

- 5: CG_l: setting up Schur red-black preconditioned CG for DWF
- 15: QZ2_l: computing quark propagator using Z2 source
- 16: meson_Z2_ll: computing meson correlators


```

408 template<class Impl>
409 void PartialFractionFermion5D<Impl>::ExportPhysicalFermionSolution(const FermionField &solution5d, FermionField &exported4d)
410
411     int Ls = this->Ls;
412     conformable(solution5d.Grid(), this->FermionGrid());
413     conformable(exported4d.Grid(), this->GaugeGrid());
414     ExtractSlice(exported4d, solution5d, Ls-1, Ls-1);
415 }

```

```

656 template<class vobj>
657 void ExtractSlice(Lattice<vobj> &lowDim, const Lattice<vobj> & higherDim, int slice, int orthog)
658 {
659     typedef typename vobj::scalar_object sobj;
660
661     GridBase *lg = lowDim.Grid();
662     GridBase *hg = higherDim.Grid();
663     int nl = lg->_ndimension;
664     int nh = hg->_ndimension;
665
666     assert(nl+1 == nh);
667     assert(orthog<nh);
668     assert(orthog>=0);
669     assert(hg->_processors[orthog]==1);
670
671     int dl; dl = 0;
672     for(int d=0; d<nh; d++){
673         if ( d != orthog) {
674             assert(lg->_processors[dl] == hg->_processors[d]);
675             assert(lg->_ldimensions[dl] == hg->_ldimensions[d]);
676             dl++;
677         }
678     }
679     // the above should guarantee that the operations are local
680     autoView(lowDimv, lowDim, CpuWrite);
681     autoView(higherDimv, higherDim, CpuRead);
682     thread_for(idx, lg->lSites(), {
683         sobj s;
684         Coordinate lcoor(nl);
685         Coordinate hcoor(nh);
686         lg->LocalIndexToLocalCoor(idx, lcoor);
687         int ddl=0;
688         hcoor[orthog] = slice;
689         for(int d=0; d<nh; d++){
690             if ( d!=orthog ) {
691                 hcoor[d]=lcoor[ddl++];
692             }
693         }
694         peekLocalSite(s, higherDimv, hcoor);
695         pokeLocalSite(s, lowDimv, lcoor);
696     });
697 }

```


Output file:

```
499 Hadrons : Message : 65.331207 s : ----- Measurement step 15/17 (module 'QZ2_l'
) -----
500 Hadrons : Message : 65.331216 s : ..... Module execution
501 Hadrons : Message : 65.331259 s : Computing quark propagator 'QZ2_l'
502 Hadrons : Message : 65.331271 s : Using source 'Z2'
503 Hadrons : Message : 65.331284 s : Inverting using solver 'CG_l'
504 Hadrons : Message : 65.331291 s : Inversion for spin= 0, color= 0
505 Hadrons : Message : 65.331297 s : Import source
506 Hadrons : Message : 65.338548 s : Solve
507 Grid : Message : 67.852095 s : ConjugateGradient Converged on iteration 318 Computed r
esidual 9.5689e-09 True residual 9.5689e-09 Target 1e-08
508 Grid : Message : 67.860724 s : SchurRedBlackBase solver true unprec resid 3.25679e-08
509 Hadrons : Message : 67.860793 s : Export solution
510 Hadrons : Message : 67.879502 s : Inversion for spin=0, color= 1
511 Hadrons : Message : 67.879525 s : Import source
512 Hadrons : Message : 67.886553 s : Solve
513 Grid : Message : 70.410080 s : ConjugateGradient Converged on iteration 319 Computed r
esidual 9.62417e-09 True residual 9.62417e-09 Target 1e-08
514 Grid : Message : 70.418756 s : SchurRedBlackBase solver true unprec resid 3.23147e-08
515 Hadrons : Message : 70.418829 s : Export solution
516 Hadrons : Message : 70.437594 s : Inversion for spin=0, color= 2
517 Hadrons : Message : 70.437619 s : Import source
518 Hadrons : Message : 70.444636 s : Solve
519 Grid : Message : 72.932850 s : ConjugateGradient Converged on iteration 314 Computed r
esidual 9.68155e-09 True residual 9.68155e-09 Target 1e-08
520 Grid : Message : 72.941565 s : SchurRedBlackBase solver true unprec resid 3.30696e-08
521 Hadrons : Message : 72.941636 s : Export solution
```


Output file:

```
589 Hadrons : Message : 95.613402 s : ----- Measurement step 16/17 (module 'meson_Z2_ll') -----
-----
590 Hadrons : Message : 95.613410 s : ..... Module execution
591 Hadrons : Message : 95.613429 s : Computing meson contractions meson_Z2_ll' using quarks 'QZ2_l' and 'Q
Z2_l'
592 Hadrons : Message : 95.613522 s : (using sink 'sink')
593 Hadrons : Message : 96.161033 s : ..... Timings
594 Hadrons : Message : 96.161071 s : * GLOBAL TIMERS
595 Hadrons : Message : 96.161082 s : total: 547606 us (100.0%)
596 Hadrons : Message : 96.161098 s : execution: 547594 us (100.0%)
597 Hadrons : Message : 96.161110 s : setup: 9 us (0.0%)
598 Hadrons : Message : 96.161124 s : ..... Memory management
599 Hadrons : Message : 96.161198 s : Memory: current total 68.1 MB / environment 464.0 MB / comms 1 GB / gr
id 464.9 MB / peak total 68.1 MB
600 Hadrons : Message : 96.161222 s : Garbage collection
601 Hadrons : Message : 96.161229 s : Destroying object 'sink'
602 Hadrons : Message : 96.161238 s : Destroying object 'QZ2_l'
603 Hadrons : Message : 96.161249 s : Destroying object 'meson_Z2_ll_tmp_c'
604 Hadrons : Message : 96.161303 s : Memory: current total 68.1 MB / environment 441.1 MB / comms 1 GB / gr
id 442.0 MB / peak total 68.1 MB
```


- `./application-template/par-example.xml:37:`
`<!-- run id (is part of seed for random numbers!) -->`

./Hadrons/Module.cpp

```
94 // make module unique string //////////////////////////////////////
95 std::string ModuleBase::makeSeedString(void)
96 {
97     std::string seed;
98
99     if (!vm().getRunId().empty())
100     {
101         seed += vm().getRunId() + "-";
102     }
103     seed += getName() + "-" + std::to_string(vm().getTrajectory());
104
105     return seed;
106 }
107
108 // get RNGs seeded from module string //////////////////////////////////
109 GridParallelRNG & ModuleBase::rng4d(void)
110 {
111     auto &r = *env().get4dRng();
112
113     if (makeSeedString() != seed_)
114     {
115         seed_ = makeSeedString();
116         LOG(Message) << "Seeding 4D RNG " << &r << " with string '"
117             << seed_ << "'" << std::endl;
118         r.SeedUniqueString(seed_);
119     }
120
121     return r;
122 }
123
```

```
308 Hadrons : Message : 4149.724463 s : ----- Measurement step 8/13 (module
      'Z2Stochastic') -----
309 Hadrons : Message : 4149.724471 s : ..... Module execution
310 Hadrons : Message : 4149.730130 s : Seeding 4D RNG 0x51bc900 with string 'test0-Z2S
      tochastic-1000'
311 Grid : Message : 4149.730170 s : Initialising parallel RNG with unique string 'te
      st0-Z2Stochastic-1000'
312 Grid : Message : 4149.730179 s : Seed SHA256: 3c1ad6cccc9e9b4fa263048ebaa3673230
      54a5ecd148a21fa2d2f064c72917
```


./Hadrons/VirtualMachine.cpp

```
867 // genetic scheduler //////////////////////////////////////
868 VirtualMachine::Program VirtualMachine::schedule(const GeneticPar &par)
869 {
870     typedef GeneticScheduler<Size, unsigned int> Scheduler;
871
872     auto graph = getModuleGraph();
873
874     //constrained topological sort using a genetic algorithm
875     LOG(Message) << "Scheduling computation" << std::endl;
876     LOG(Message) << "#module=" << graph.size() << std::endl;
877     LOG(Message) << "population size=" << par.popSize << std::endl;
878     LOG(Message) << "max. generation=" << par.maxGen << std::endl;
879     LOG(Message) << "max. cst. generation=" << par.maxCstGen << std::endl;
880     LOG(Message) << "mutation rate=" << par.mutationRate << std::endl;
881
882     unsigned int gen, prevPeak, nCstPeak = 0;
883     std::random_device rd;
884     Scheduler::Parameters gpar;
885
886     gpar.popSize = par.popSize;
887     gpar.mutationRate = par.mutationRate;
888     gpar.seed = rd();
889     CartesianCommunicator::BroadcastWorld(0, &(gpar.seed), sizeof(gpar.seed));
```

```
63 Hadrons : Message : 3.271217 s : ===== HADRONS APPLICATION START =====
64 Hadrons : Message : 3.271232 s : RUN ID 'test0'
65 Hadrons : Message : 3.271239 s : Attempt(s) for resilient parallel I/O: -1
66 Hadrons : Message : 3.271320 s : Logging run statistics in 'test0-stat-20211018-175
822.db'
67 Hadrons : Message : 3.409232 s : Scheduling computation...
68 Hadrons : Message : 3.409253 s : #module= 13
69 Hadrons : Message : 3.409260 s : population size= 20
70 Hadrons : Message : 3.409266 s : max. generation= 1000
71 Hadrons : Message : 3.409272 s : max. cst. generation= 100
72 Hadrons : Message : 3.409278 s : mutation rate= 0.1
73 Hadrons : Message : 5.350401 s : Start: 733.8 MB
74 Hadrons : Message : 5.351056 s : Generation 0: 703.6 MB
75 Hadrons : Message : 5.356127 s : Generation 10: 703.6 MB
76 Hadrons : Message : 5.361496 s : Generation 20: 703.6 MB
77 Hadrons : Message : 5.366835 s : Generation 30: 703.6 MB
78 Hadrons : Message : 5.371969 s : Generation 40: 703.6 MB
79 Hadrons : Message : 5.377149 s : Generation 50: 703.6 MB
80 Hadrons : Message : 5.382757 s : Generation 60: 703.6 MB
81 Hadrons : Message : 5.387961 s : Generation 70: 703.6 MB
82 Hadrons : Message : 5.393821 s : Generation 80: 703.6 MB
83 Hadrons : Message : 5.399349 s : Generation 90: 703.6 MB
84 Hadrons : Message : 5.404762 s : Generation 100: 703.6 MB
85 Hadrons : Message : 5.406637 s : Schedule (memory needed: 703.6 MB):
```



```

470 //template <class Prop, class Ferm>
471 template <class Fimpl>
472 void PropToFerm(typename Fimpl::FermionField &f, const typename Fimpl::PropagatorField &p, const int s, const int c)
473 {
474     for(int j = 0; j < Ns; ++j)
475     {
476         auto pjs = peekSpin(p, j, s);
477         auto fj = peekSpin(f, j);
478
479         for(int i = 0; i < Fimpl::Dimension; ++i)
480         {
481             pokeColour(fj, peekColour(pjs, i, c), i);
482         }
483         pokeSpin(f, fj, j);
484     }
485 }

```

$$pjs = \text{peekSpin}(p, j, s) : pjs = p_{js}; \quad fj = \text{peekSpin}(f, j) : fj = f_j$$

$$\text{peekColour}(pjs, i, c) : p_{js}; \quad \text{pokeColour}(fj, \text{peekColour}(pjs, i, c), i) : f_{j_i} = p_{js_{ic}}$$

$$\text{pokeSpin}(f, fj, j) : f_j = f_j$$


```
64 int Environment::getDim(const unsigned int mu) const
65 {
66     return dim_[mu];
67 }
68
```

```
42 Environment::Environment(void)
43 {
44     dim_ = GridDefaultLatt().toVector();
45     nd_ = dim_.size();
46     vol_ = 1.;
47     for (auto d: dim_)
48     {
49         vol_ *= d;
50     }
51 }
```

15.2 Grid Initialization

Grid itself is initialized with a call:

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

Command line options include:

```
--mpi n.n.n.n : default MPI decomposition  
--threads n : default number of OMP threads  
--grid n.n.n.n : default Grid size
```

where *argc* and *argv* are constructed to simulate the command-line options described above. At a minimum one usually provides the *-grid* and *-mpi* parameters. The former specifies the lattice dimensions and the latter specifies the grid of processors (MPI ranks). If these parameters are not specified with the *Grid_init* call, they need to be supplied later when creating Grid fields.

The following Grid procedures are useful for verifying that Grid “default” values are properly initialized.

Grid procedure	returns
<code>std::vector<int> GridDefaultLatt();</code>	lattice size
<code>std::vector<int> GridDefaultSimd(int Nd,vComplex::Nsimd());</code>	SIMD layout
<code>std::vector<int> GridDefaultMpi();</code>	MPI layout
<code>int Grid::GridThread::GetThreads();</code>	number of threads

Code running procedure

utilities/HadronsXmlRun.cpp

```
32 int main(int argc, char *argv[])
33
34 // parse command line
35 std::string parameterFileName;
36
37 if (argc < 2)
38 {
39     std::cerr << "usage: " << argv[0] << " <parameter file> [Grid options]";
40     std::cerr << std::endl;
41     std::exit(EXIT_FAILURE);
42 }
43 parameterFileName = argv[1];
44
45 // initialization
46 Grid_init(&argc, &argv);
47
48 // execution
49 try
50 {
51     Application application(parameterFileName);
52     application.parseParameterFile(parameterFileName);
53     application.run();
54 }
55 catch (const std::exception& e)
56 {
57     Exceptions::abort(e);
58 }
59
60
61 // epilogue
62 LOG(Message) << "Grid is finalizing now" << std::endl;
63 Grid_finalize();
64
65 return EXIT_SUCCESS;
66
```

The main function of every GRID program starts with an initialization `Grid_init()` and ends with the corresponding `Grid_finalize()` function call

Application.cpp

```
222 // parse parameter file //////////////////////////////////////
223 void Application::parseParameterFile(const std::string parameterFileName)
224 {
225     XmlReader reader(parameterFileName, false, HADRONS_XML_TOPLEV);
226     GlobalPar par;
227     ObjectId id;
228
229     LOG(Message) << "Building application from '" << parameterFileName << "'";
230     read(reader, "parameters", par);
231     setPar(par);
232     if (!par.database.restoreModules)
233     {
234         if (!push(reader, "modules"))
235         {
236             HADRONS_ERROR(Parsing, "Cannot open node 'modules' in parameter file '"
237                 + parameterFileName + "'");
238         }
239         if (!push(reader, "module"))
240         {
241             HADRONS_ERROR(Parsing, "Cannot open node 'modules/module' in parameter file '"
242                 + parameterFileName + "'");
243         }
244         do
245         {
246             read(reader, "id", id);
247             createModule(id.name, id.type, reader);
248         } while (reader.nextElement("module"));
249         pop(reader);
250         pop(reader);
251     }
252     else
253     {
254         LOG(Message) << "XML module list ignored (restored from database '"
255             << par.database.applicationDb << "')";
256     }
257 }
```


Application.cpp

```
155 // execute //////////////////////////////////////
156 void Application::run(void)
157 {
158     Database statDb;
159     StatLogger statLogger;
160
161     LOG(Message) << "==== HADRONS APPLICATION START ====" << std::endl;
162     if (!parameterFileName_.empty() and (vm().getNModule() == 0))
163     {
164         parseParameterFile(parameterFileName_);
165     }
166     if (getPar().runId.empty())
167     {
168         HADRONS_ERROR(Definition, "run id is empty");
169     }
170     LOG(Message) << "RUN ID '" << getPar().runId << "'" << std::endl;
171     BinaryIO::latticeWriteMaxRetry = getPar().parallelWriteMaxRetry;
172     LOG(Message) << "Attempt(s) for resilient parallel I/O: "
173         << BinaryIO::latticeWriteMaxRetry << std::endl;
174     vm().setRunId(getPar().runId);
175     if (getPar().database.makeStatDb)
176     {
177         std::string statDbFilename;
178         std::ostringstream oss;
179         auto now = std::chrono::system_clock::to_time_t(std::chrono::system_clock::now());
180         auto nowLocal = *std::localtime(&now);
181
182         oss << std::put_time(&nowLocal, "%Y%m%d-%H%M%S");
183         statDbFilename = getPar().runId + "-stat-" + oss.str() + ".db";
184         LOG(Message) << "Logging run statistics in '" << statDbFilename << "'" << std::endl;
185         if (env().getGrid()->IsBoss())
186         {
187             statDb.setFilename(statDbFilename);
188             statLogger.setDatabase(statDb);
189             statLogger.start(500);
190         }
191     }
```


Application.cpp

```
192     if (getPar().saveSchedule or getPar().scheduleFile.empty())
193     {
194         schedule();
195         if (getPar().saveSchedule)
196         {
197             std::string filename;
198
199             filename = (getPar().scheduleFile.empty()) ?
200                 "hadrons.sched" : getPar().scheduleFile;
201             saveSchedule(filename);
202         }
203     }
204     else
205     {
206         loadSchedule(getPar().scheduleFile);
207     }
208     printSchedule();
209     vm().printMemoryProfile();
210     if (!getPar().graphFile.empty())
211     {
212         makeFileDir(getPar().graphFile, env().getGrid());
213         vm().dumpModuleGraph(getPar().graphFile);
214     }
215     configLoop();
216     if (getPar().database.makeStatDb and env().getGrid()->IsBoss())
217     {
218         statLogger.stop();
219     }
220 }
```

VirtualMachine.cpp

```
867 // genetic scheduler //////////////////////////////////////
868 VirtualMachine::Program VirtualMachine::schedule(const GeneticPar &par)
869 {
870     typedef GeneticScheduler<Size, unsigned int> Scheduler;
871
872     auto graph = getModuleGraph();
873
874     //constrained topological sort using a genetic algorithm
875     LOG(Message) << "Scheduling computation..." << std::endl;
876     LOG(Message) << "    #module= " << graph.size() << std::endl;
877     LOG(Message) << "    population size= " << par.popSize << std::endl;
878     LOG(Message) << "    max. generation= " << par.maxGen << std::endl;
879     LOG(Message) << "    max. cst. generation= " << par.maxCstGen << std::endl;
880     LOG(Message) << "    mutation rate= " << par.mutationRate << std::endl;
881
882     unsigned int gen, prevPeak, nCstPeak = 0;
883     std::random_device rd;
884     Scheduler::Parameters gpar;
885
886     gpar.popSize = par.popSize;
887     gpar.mutationRate = par.mutationRate;
888     gpar.seed = rd();
889     CartesianCommunicator::BroadcastWorld(0, &(gpar.seed), sizeof(gpar.seed));
890     Scheduler::ObjFunc memPeak = [this](const Program &p) ->Size
891     {
892         return memoryNeeded(p);
893     };
894     Scheduler scheduler(graph, memPeak, gpar);
895     gen = 0;
896     scheduler.initPopulation();
897     LOG(Message) << "Start: " << sizeString(scheduler.getMinValue())
898         << std::endl;
899     do
```


VirtualMachine.cpp

```
899 do
900 {
901     scheduler.nextGeneration();
902     if (gen != 0)
903     {
904         if (prevPeak == scheduler.getMinValue())
905         {
906             nCstPeak++;
907         }
908         else
909         {
910             nCstPeak = 0;
911         }
912     }
913     prevPeak = scheduler.getMinValue();
914     if (gen % 10 == 0)
915     {
916         LOG(Message) << "Generation " << gen << ": "
917             << sizeString(scheduler.getMinValue()) << std::endl;
918     }
919     gen++;
920 } while ((gen < par.maxGen) and (nCstPeak < par.maxCstGen));
921 if (hasDatabase() and makeScheduleDb_)
922 {
923     Program p = scheduler.getMinSchedule();
924     for (unsigned int i = 0; i < p.size(); ++i)
925     {
926         ScheduleEntry s;
927         s.step = i;
928         s.moduleId = p[i];
929         db_>insert("schedule", s);
930     }
931 }
932 return scheduler.getMinSchedule();
933 }
```

Application.cpp

```
334 void Application::printSchedule(void)
335 {
336     if (!scheduled_ and !loadedSchedule_)
337     {
338         HADRON_ERROR(Definition, "Computation not scheduled");
339     }
340     auto peak = vm().memoryNeeded(program_);
341     LOG(Message) << "Schedule (memory needed: " << sizeString(peak) << "):"
342         << std::endl;
343     for (unsigned int i = 0; i < program_.size(); ++i)
344     {
345         LOG(Message) << std::setw(4) << i + 1 << ": "
346             << vm().getModuleName(program_[i]) << std::endl;
347     }
348 }
```


Application.cpp

```
350 // loop on configurations ////////////////////////////////////////
351 void Application::configLoop(void)
352 {
353     auto range = par_.trajCounter;
354
355     for (unsigned int t = range.start; t < range.end; t += range.step)
356     {
357         LOG(Message) << BIG_SEP << " Starting measurement for trajectory " << t
358             << " " << BIG_SEP << std::endl;
359         vm().setTrajectory(t);
360         vm().executeProgram(program_);
361     }
362     LOG(Message) << BIG_SEP << " End of measurement " << BIG_SEP << std::endl;
363     env().freeAll();
364 }
```


VirtualMachine.cpp

```
1030 void VirtualMachine::executeProgram(const std::vector<std::string> &p)
1031 {
1032     Program pAddress;
1033
1034     for (auto &n: p)
1035     {
1036         pAddress.push_back(getModuleAddress(n));
1037     }
1038     executeProgram(pAddress);
1039 }
```

```
945 void VirtualMachine::executeProgram(const Program &p)
946 {
947     Size memPeak = 0, sizeBefore, sizeAfter;
948     GarbageSchedule freeProg;
949
950     // build garbage collection schedule
951     LOG(Debug) << "Building garbage collection schedule..." << std::endl;
952     freeProg = makeGarbageSchedule(p);
953     for (unsigned int i = 0; i < freeProg.size(); ++i)
954     {
955         std::string msg = "";
956
957         for (auto &a: freeProg[i])
958         {
959             msg += env().getObjectName(a) + " ";
960         }
961         msg += " ]";
962         LOG(Debug) << std::setw(4) << i + 1 << ": [" << msg << std::endl;
963     }
964
965     // program execution
966     LOG(Debug) << "Executing program..." << std::endl;
967     totalTime_ = GridTime::zero();
968     for (unsigned int i = 0; i < p.size(); ++i)
969     {
970         // execute module
971         LOG(Message) << SEP << " Measurement step " << i + 1 << "/"
972             << p.size() << " (module '" << module_[p[i]].name
973             << "') " << SEP << std::endl;
974         LOG(Message) << SMALL_SEP << " Module execution" << std::endl;
975         currentModule = p[i];
976         (*module_[p[i]].data());
977         currentModule_ = -1;
978         sizeBefore = env().getTotalSize();
979         // print time profile after execution
980         LOG(Message) << SMALL_SEP << " Timings" << std::endl;
981
982         std::map<std::string, GridTime> ctiming, gtiming;
983         GridTime total;
984     }
```


VirtualMachine.cpp

```
985     ctiming = module_[p[i]].data->getTimings();
986     total   = ctiming.at("_total");
987     gtiming["total"] = ctiming["_total"];   ctiming.erase("_total");
988     gtiming["setup"] = ctiming["_setup"];   ctiming.erase("_setup");
989     gtiming["execution"] = ctiming["_execute"]; ctiming.erase("_execute");
990     LOG(Message) << "* GLOBAL TIMERS" << std::endl;
991     printTimeProfile(gtiming, total);
992     if (!ctiming.empty())
993     {
994         LOG(Message) << "* CUSTOM TIMERS" << std::endl;
995         printTimeProfile(ctiming, total);
996     }
997     timeProfile_[module_[p[i]].name] = total;
998     totalTime_ += total;
999     // print used memory after execution
1000    LOG(Message) << SMALL_SEP << " Memory management" << std::endl;
1001    MemoryUtils::printMemory();
1002    if (sizeBefore > memPeak)
1003    {
1004        memPeak = sizeBefore;
1005    }
1006    // garbage collection for step i
1007    LOG(Message) << "Garbage collection..." << std::endl;
1008    for (auto &j: freeProg[i])
1009    {
1010        env().freeObject(j);
1011    }
1012    // print used memory after garbage collection if necessary
1013    sizeAfter = env().getTotalSize();
1014    if (sizeBefore != sizeAfter)
1015    {
1016        MemoryUtils::printMemory();
1017    }
1018    else
1019    {
1020        LOG(Message) << "Nothing to free" << std::endl;
1021    }
1022 }
1023 // print total time profile
1024 LOG(Message) << SEP << " Measurement time profile" << SEP << std::endl;
1025 LOG(Message) << "Total measurement time: " << totalTime_ << " us" << std::endl;
1026 LOG(Message) << SMALL_SEP << " Module breakdown" << std::endl;
1027 printTimeProfile(timeProfile_, totalTime_);
1028 }
```


Modules/MSink/Point.hpp

```
120 // execution //////////////////////////////////////
121 template <typename Field>
122 void TPoint<Field>::execute(void)
123 {
124     LOG(Message) << "Setting up point sink function for momentum ["
125                 << par().mom << "]" << std::endl;
126
127     auto &ph = envGet(LatticeComplex, momphName_);
128
129     if (!hasPhase_)
130     {
131         Complex          i(0.0,1.0);
132         std::vector<Real> p;
133
134         envGetTmp(LatticeComplex, coor);
135         p = strToVec<Real>(par().mom);
136         ph = Zero();
137         for(unsigned int mu = 0; mu < p.size(); mu++)
138         {
139             LatticeCoordinate(coor, mu);
140             ph = ph + (p[mu]/env().getDim(mu))*coor;
141         }
142         ph = exp((Real)(2*M_PI)*i*ph);
143         hasPhase_ = true;
144     }
145     auto sink = [this](const PropagatorField &field)
146     {
147         SlicedPropagator res;
148         auto &ph = envGet(LatticeComplex, momphName_);
149         PropagatorField tmp = ph*field;
150
151         sliceSum(tmp, res, Tp);
152
153         return res;
154     };
155     envGet(SinkFn, getName()) = sink;
156 }
```


Modules/MIO/LoadNersc.hpp

```
101 // execution //////////////////////////////////////
102 template <typename GImpl>
103 void TLoadNersc<GImpl>::execute(void)
104 {
105     FieldMetaData header;
106     std::string fileName = par().file + "."
107         + std::to_string(vm().getTrajectory());
108     LOG(Message) << "Loading NERSC configuration from file" << fileName
109         << "" << std::endl;
110
111     auto &U = envGet(GaugeField, getName());
112     NerscIO::readConfiguration(U, header, fileName);
113 }
114
```


Hadrons/Modules/MGauge/StoutSmearing.hpp

```
104 // execution //////////////////////////////////////
105 template <typename GImpl>
106 void TStoutSmearing<GImpl>::execute(void)
107 {
108     LOG(Message) << "Smearing " << par().gauge << " with " << par().steps
109     << " step" << ((par().steps > 1) ? "s" : "")
110     << " of stout smearing and rho=" << par().rho << std::endl;
111
112     Smear_Stout<GImpl> smearer(par().rho);
113     auto &U = envGet(GaugeField, par().gauge);
114     auto &Usmr = envGet(GaugeField, getName());
115
116     envGetTmp(GaugeField, buf);
117     buf = U;
118     LOG(Message) << "plaquette=" << WilsonLoops<GImpl>::avgPlaquette(U)
119     << std::endl;
120     for (unsigned int n = 0; n < par().steps; ++n)
121     {
122         smearer.smear(Usmr, buf);
123         buf = Usmr;
124         LOG(Message) << "plaquette=" << WilsonLoops<GImpl>::avgPlaquette(Usmr)
125         << std::endl;
126     }
127 }
```


Hadrons/Modules/MAction/ScaledDWF.hpp

```
103 // setup //////////////////////////////////////
104 template <typename FImpl>
105 void TScaledDWF<FImpl>::setup(void)
106 {
107     LOG(Message) << "Setting up scaled domain wall fermion matrix with m= "
108                 << par().mass << ", M5= " << par().M5 << ", Ls= " << par().Ls
109                 << ", scale= " << par().scale
110                 << " using gauge field '" << par().gauge << "'"
111                 << std::endl;
112
113     auto &U    = envGet(GaugeField, par().gauge);
114     auto &g4    = *envGetGrid(FermionField);
115     auto &grb4 = *envGetRbGrid(FermionField);
116     auto &g5    = *envGetGrid(FermionField, par().Ls);
117     auto &grb5 = *envGetRbGrid(FermionField, par().Ls);
118     typename ScaledShamirFermion<FImpl>::ImplParams implParams;
119     if (!par().boundary.empty())
120     {
121         implParams.boundary_phases = strToVec<Complex>(par().boundary);
122     }
123     if (!par().twist.empty())
124     {
125         implParams.twist_n_2pi_L = strToVec<Real>(par().twist);
126     }
127     LOG(Message) << "Fermion boundary conditions: " << implParams.boundary_phases
128                 << std::endl;
129     LOG(Message) << "Twists: " << implParams.twist_n_2pi_L
130                 << std::endl;
131     if (implParams.boundary_phases.size() != env().getNd())
132     {
133         HADRONS_ERROR(Size, "Wrong number of boundary phase");
134     }
135     if (implParams.twist_n_2pi_L.size() != env().getNd())
136     {
137         HADRONS_ERROR(Size, "Wrong number of twist");
138     }
139     envCreateDerived(FMat, ScaledShamirFermion<FImpl>, getName(), par().Ls, U, g5,
140                    grb5, g4, grb4, par().mass, par().M5, par().scale,
141                    implParams);
142 }
143 // execution //////////////////////////////////////
144 template <typename FImpl>
145 void TScaledDWF<FImpl>::execute(void)
146 {}
```


Hadrons/Modules/MSolver/RBPreCG.hpp

```
119 // setup //////////////////////////////////////
120 template <typename FImpl, int nBasis>
121 void TRBPreCG<FImpl, nBasis>::setup(void)
122 {
123     if (par().maxIteration == 0)
124     {
125         HADRONS_ERROR(Argument, "zero maximum iteration");
126     }
127
128     LOG(Message) << "setting up Schur red-black preconditioned CG for"
129                 << " action '" << par().action << "' with residual"
130                 << par().residual << ", maximum iteration"
131                 << par().maxIteration << std::endl;
132
133     auto Ls = env().getObjectLs(par().action);
134     auto &mat = envGet(FMat, par().action);
135     auto guesserPt = makeGuesser<FImpl, nBasis>(par().eigenPack);
136
137     auto makeSolver = [&mat, guesserPt, this](bool subGuess)
138     {
139         return [&mat, guesserPt, subGuess, this](FermionField &sol,
140         const FermionField &source)
141         {
142             ConjugateGradient<FermionField> cg(par().residual,
143             par().maxIteration);
144             HADRONS_DEFAULT_SCHUR_SOLVE<FermionField> schurSolver(cg);
145             schurSolver.subtractGuess(subGuess);
146             schurSolver(mat, source, sol, *guesserPt);
147         };
148     };
149
150     auto solver = makeSolver(false);
151     envCreate(Solver, getName(), Ls, solver, mat);
152     auto solver_subtract = makeSolver(true);
153     envCreate(Solver, getName() + "_subtract", Ls, solver_subtract, mat);
154 }
155
156 // execution //////////////////////////////////////
157 template <typename FImpl, int nBasis>
158 void TRBPreCG<FImpl, nBasis>::execute(void)
159 {}
```


Hadrons/Modules/MSource/Z2.hpp

```
125 // execution //////////////////////////////////////
126 template <typename FImpl>
127 void TZ2<FImpl>::execute(void)
128 {
129     if (par().tA == par().tB)
130     {
131         LOG(Message) << "Generating Z_2 wall source at t=" << par().tA
132             << std::endl;
133     }
134     else
135     {
136         LOG(Message) << "Generating Z_2 band for " << par().tA << " " << par().tB << std::endl;
137     }
138 }
139
140 auto &src = envGet(PropagatorField, getName());
141 auto &t = envGet(Lattice<iScalar<vInteger>>, tName);
142 Complex shift(1., 1.);
143
144 if (!hasT_)
145 {
146     LatticeCoordinate(t, Tp);
147     hasT_ = true;
148 }
149 envGetTmp(LatticeComplex, eta);
150 bernoulli(rng4d(), eta);
151 eta = (2.*eta - shift)*(1./::sqrt(2.));
152 eta = where((t >= par().tA) and (t <= par().tB), eta, 0.*eta);
153 src = 1.;
154 src = src*eta;
155 }
```


Hadrons/Modules/MFermion/GaugeProp.hpp

```
216 template <typename FImpl>
217 void TGaugeProp<FImpl>::execute(void)
218 {
219     LOG(Message) << "Computing quark propagator '" << getName() << "'
220         << std::endl;
221
222     std::string propName = (Ls_ == 1) ? getName() : (getName() + "_5d");
223
224     if (envHasType(PropagatorField, par().source))
225     {
226         auto &prop = envGet(PropagatorField, propName);
227         auto &propPhysical = envGet(PropagatorField, getName());
228         auto &fullSrc = envGet(PropagatorField, par().source);
229
230         LOG(Message) << "Using source '" << par().source << "' << std::endl;
231         solvePropagator(prop, propPhysical, fullSrc);
232     }
233     else
234     {
235         auto &prop = envGet(std::vector<PropagatorField>, propName);
236         auto &propPhysical = envGet(std::vector<PropagatorField>, getName());
237         auto &fullSrc = envGet(std::vector<PropagatorField>, par().source);
238
239         for (unsigned int i = 0; i < fullSrc.size(); ++i)
240         {
241             LOG(Message) << "Using element " << i << " of source vector '"
242                 << par().source << "' << std::endl;
243             solvePropagator(prop[i], propPhysical[i], fullSrc[i]);
244         }
245     }
246 }
```


Hadrons/Modules/MFermion/GaugeProp.hpp

```
157 // execution //////////////////////////////////////
158 template <typename FImpl>
159 void TGaugeProp<FImpl>::solvePropagator(PropagatorField &prop,
160                                         PropagatorField &propPhysical,
161                                         const PropagatorField &fullSrc)
162 {
163     auto & solver = envGet(Solver, par().solver);
164     auto & mat = solver.getFMat();
165
166     envGetTmp(FermionField, source);
167     envGetTmp(FermionField, sol);
168     envGetTmp(FermionField, tmp);
169     LOG(Message) << "Inverting using solver " << par().solver << "
170                 << std::endl;
171     for (unsigned int s = 0; s < Ns; ++s)
172     for (unsigned int c = 0; c < FImpl::Dimension; ++c)
173     {
174         LOG(Message) << "Inversion for spin= " << s << ", color= " << c
175                 << std::endl;
176         // source conversion for 4D sources
177         LOG(Message) << "Import source" << std::endl;
178         if (!env().isObject5d(par().source))
179         {
180             if (Ls_ == 1)
181             {
182                 PropToFerm<FImpl>(source, fullSrc, s, c);
183             }
184         }
185     }
186     else
187     {
188         PropToFerm<FImpl>(tmp, fullSrc, s, c);
189         mat.ImportPhysicalFermionSource(tmp, source);
190     }
191 }
```

```
190 // source conversion for 5D sources
191 else
192 {
193     if (Ls_ != env().getObjectLs(par().source))
194     {
195         HADRONS_ERROR(Size, "Ls mismatch between quark action and source");
196     }
197     else
198     {
199         PropToFerm<FImpl>(source, fullSrc, s, c);
200     }
201 }
202 sol = Zero();
203 LOG(Message) << "Solve" << std::endl;
204 solver(sol, source);
205 LOG(Message) << "Export solution" << std::endl;
206 FermToProp<FImpl>(prop, sol, s, c);
207 // create 4D propagators from 5D one if necessary
208 if (Ls_ > 1)
209 {
210     mat.ExportPhysicalFermionSolution(sol, tmp);
211     FermToProp<FImpl>(propPhysical, tmp, s, c);
212 }
213 }
214 }
```


Hadrons/Modules/MContraction/Meson.hpp

```
// execution //////////////////////////////////////
#define mesonConnected(q1, q2, gSnk, gSrc) \
(g5*(gSnk))*(q1)*(adj(gSrc)*g5)*adj(q2)
template <typename FImpl1, typename FImpl2>
void TMeson<FImpl1, FImpl2>::execute(void)
{
    LOG(Message) << "Computing meson contractions " << getName() << " using "
    << " quarks " << par().q1 << " and " << par().q2 << " if "
    << std::endl;

    std::vector<TComplex> buf;
    std::vector<Result> result;
    Gamma g5(Gamma::Algebra::Gamma5);
    std::vector<GammaPair> gammaList;
    int nt = env().getDim(Tp);

    parseGammaString(gammaList);
    result.resize(gammaList.size());
    for (unsigned int i = 0; i < result.size(); ++i)
    {
        result[i].gamma_snk = gammaList[i].first;
        result[i].gamma_src = gammaList[i].second;
        result[i].corr.resize(nt);
    }
}
```

$g_{Snk}, g_{Src} \in \Gamma_i (i = 0, 1, \dots, 15)$

$t = 0, 1, \dots, N_t - 1$

q_1, q_2 are quark propagators

```
auto &q1 = envGet(PropagatorField1, par().q1);
auto &q2 = envGet(PropagatorField2, par().q2);

envGetTmp(LatticeComplex, c);
LOG(Message) << "(using sink '" << par().sink << "')" << std::endl;
for (unsigned int i = 0; i < result.size(); ++i)
{
    Gamma gSnk(gammaList[i].first);
    Gamma gSrc(gammaList[i].second);
    std::string ns;

    ns = vm().getModuleNamespace(env().getObjectModule(par().sink));
    if (ns == "MSource")
    {
        PropagatorField1 &sink = envGet(PropagatorField1, par().sink);

        c = trace(mesonConnected(q1, q2, gSnk, gSrc)*sink);
        sliceSum(c, buf, Tp);
    }
    else if (ns == "MSink")
    {
        SinkFnScalar &sink = envGet(SinkFnScalar, par().sink);

        c = trace(mesonConnected(q1, q2, gSnk, gSrc)*sink);
        buf = sink(c);
    }
    for (unsigned int t = 0; t < buf.size(); ++t)
    {
        result[i].corr[t] = TensorRemove(buf[t]);
    }
}

saveResult(par().output, "meson", result);
```


Hadrons/Modules/MContraction/WardIdentity.hpp

```
160 // execution //////////////////////////////////////
161 template <typename FImpl>
162 void TWardIdentity<FImpl>::execute(void)
163 {
164     LOG(Message) << "Performing Ward Identity checks for propagator " << par().prop << std::endl;
165     auto &prop = envGet(PropagatorField, par().prop);
166     LOG(Message) << "Action " << par().action << std::endl;
167     auto &act = envGet(FMat, par().action);
168     LOG(Message) << "Physical source " << par().source << std::endl;
169     auto &phys_source = envGet(PropagatorField, par().source);
170     Gamma g5(Gamma::Algebra::Gamma5);
171     Gamma gT(Gamma::Algebra::GammaT);
172
173     // Create results = zero
174     Result result;
175     result.mass = par().mass;
176     const int nt { env().getDim(Tp) };
177     result.DmuJmu.resize(nt, 0.);
178     result.VDmuJmu.resize(nt, 0.);
179     result.PJ5q.resize(nt, 0.);
180     result.PA0.resize(nt, 0.);
181
182     // Compute D_mu V_mu (D here is backward derivative)
183     // There is no point performing Dmu on spatial directions, because after the spatial sum, these become zero
184     envGetTmp(PropagatorField, tmp);
185     envGetTmp(ComplexField, tmp_current);
186     SlicedComplex sumSV(nt);
187     SlicedComplex sumVV(nt);
188     LOG(Message) << "Getting vector conserved current" << std::endl;
189     act.ContractConservedCurrent(prop, prop, tmp, phys_source, Current::Vector, Tdir);
190     // Scalar-vector current density
191     tmp_current = trace(tmp);
192     SliceOut(result.DmuJmu, sumSV, tmp_current, true);
```


Hadrons/Modules/MContraction/WardIdentity.hpp

```
193 // Vector-vector current density
194 tmp_current = trace(gT*tmp);
195 SliceOut(result.VDmuJmu, sumVV, tmp_current, true);
196 //define COMPARE_Test_Cayley_mres
197 #ifdef COMPARE_Test_Cayley_mres
198 // For comparison with Grid Test_Cayley_mres
199 LOG(Message) << "Vector Ward Identity by timeslice" << std::endl;
200 for (int t = 0; t < nt; ++t)
201 {
202     LOG(Message) << " t=" << t << ", SV=" << real(TensorRemove(sumSV[t]))
203         << ", VV=" << real(TensorRemove(sumVV[t])) << std::endl;
204 }
205 #endif
206
207 // Test axial Ward identity for 5D actions
208 if (Ls_ > 1)
209 {
210     LOG(Message) << "Getting axial conserved current" << std::endl;
211     act.ContractConservedCurrent(prop, prop, tmp, phys_source, Current::Axial, Tdir);
212     // Pseudoscalar-Axial current density
213     tmp_current = trace(g5 * tmp);
214     SlicedComplex sumPA(nt);
215     // Save temporal component of pseudoscalar-(partially) conserved axial
216     // \mathcal{A}_0 from eq (37) in https://arxiv.org/pdf/hep-lat/0612005.pdf
217     SliceOut(result.PA0, sumPA, tmp_current, false);
218     // <P|J5q>
219     act.ContractJ5q(prop, tmp_current);
220     SlicedComplex sumPJ5q(nt);
221     SliceOut(result.PJ5q, sumPJ5q, tmp_current, false);
222 }
223
224 LOG(Message) << "Writing results to " << par().output << "." << std::endl;
225 saveResult(par().output, "wardIdentity", result);
226 }
```


Module.hpp

```
98 #define envGet(type, name)\  
99 *env().template getObject<type>(name)
```

Environment.hpp

```
556 template <typename T>
557 T * Environment::getObject(const std::string name) const
558 {
559     return getObject<T>(getObjectAddress(name));
560 }
```


Environment.cpp

```
146 unsigned int Environment::getObjectAddress(const std::string name) const
147 {
148     if (hasObject(name))
149     {
150         return objectAddress_.at(name);
151     }
152     else
153     {
154         HADRON_ERROR(Definition, "no object with name " + name + "");
155     }
156 }
```

Grid/qcd/action/pseudofermion/TwoFlavour.h

```
73 ///////////////////////////////////////////////////////////////////
74 // Push the gauge field in to the dops. Assume any BC's and smearing already applied
75 ///////////////////////////////////////////////////////////////////
76 virtual void refresh(const GaugeField &U, GridSerialRNG &sRNG, GridParallelRNG &pRNG) {
77     // P(phi) = e^{- phi^dag (MdagM)^{-1} phi}
78     // Phi = Mdag eta
79     // P(eta) = e^{- eta^dag eta}
80     //
81     // e^{x^2/2 sig^2} => sig^2 = 0.5.
82     //
83     // So eta should be of width sig = 1/sqrt(2).
84     // and must multiply by 0.707....
85     //
86     // Chroma has this scale factor: two_flavor_monomial_w.h
87     // CPS uses this factor
88     // IroIro: does not use this scale. It is absorbed by a change of vars
89     //           in the Phi integral, and thus is only an irrelevant prefactor for
90     //           the partition function.
91     //
92     const RealD scale = std::sqrt(0.5);
93     FermionField eta(FermOp.FermionGrid());
94     gaussian(pRNG, eta); eta = scale *eta;
95     FermOp.ImportGauge(U);
96     FermOp.Mdag(eta, Phi);
97 };
```