Code development (not only) for NSPT

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Outline of the talk

- Motivations: NSPT
- *parmalgt* features
- Parallelization
- Some applications

- A possible strategy for parallelization of the Wilson Dirac operator

NSPT in brief

Parisi and Wu, *Perturbation Theory Without Gauge Fixing* (1981)

- introduce a new degree of freedom *"stochastic time"* $\phi(x) \to \phi(x,t)$
- let the system evolve according Langevin dynamic

$$\frac{\partial \phi(x,t)}{\partial t} = -\frac{\delta S[\phi]}{\delta \phi(x,t)} + \eta(x,t)$$

where $\eta(x,t)$ is a random noise s.t.

$$\langle \eta(x,t) \rangle = 0 \qquad \langle \eta(x,t)\eta(x',t') \rangle = 2\delta(x-x')\delta(t-t')$$

- solve the Langevin equation given some initial condition at $t = t_0$

In the case of gauge theories the resulting Langevin equation is

$$\frac{\partial}{\partial t} U(t) = \left[-i\nabla S[U] - i\eta\right] U(t)$$

Di Renzo, Marchesini, Onofri, *Numerical Stochastic Perturbation Theory* (1993)

- expand the link in power series $U_\mu = \sum_{n=0} \beta^{-n/2} U_\mu^{(n)}$
- plug the expansion in Langevin equation $\Rightarrow$ hierarchy of equations truncated at a given order
- eventually convert differential equations into integral ones

The integration is performed numerically in a perturbative MonteCarlo simulation

One can get rid of the perturbative structure of the computations by defining perturbative operations, e.g.

$$\begin{aligned} A * B &= \left\{ (A*B)^{(0)}, \beta^{-1/2}(A*B)^{(1)}, \beta^{-1}(A*B)^{(2)}, \ldots \right\} \\ (A*B)^{(ord)} &= \sum_{i=0}^{ord} A^{(i)} B^{(ord-i)} \end{aligned}$$

parmalgt

When trying to implement NSPT we had to face some difficulties:

- no simulation software exists that allows a broad flexibility for the data type stored at each lattice site;
- in order to achieve performance LQCD programs are rather difficult to read/modify;
- parallelization is hardly coded in the main routines $\Rightarrow$ trying to modify it can be a pain;

Little history

- TAO language on APE
- Cpp2 ("Enzo's code")
- PRlgt (during my PhD)

(Not) yet another simulation program. . .

parmalgt is a C++ framework which aims to be a general (not specific to QCD) environment where some 'objects' live on a D-dimensional lattice.

We're mainly interested a general environment rather than the "program" itself.

- data type flexibility (C++ templates)
  - scalar
  - gauge (any N)
  - fermions
  - . . .
- any number of physical dimension for free
- perturbative operation already coded (operator overloading)
  - on your own data type symply define basic operations
- hide involved mathematical expressions with standard symbols

Structure of the code

Different layers of code ensure modularity

- Underlying mathematics
  - complex numbers, $N \times N$ matrices, random number generator(s)
  - perturbative structures
  - physical objects: gluon, fermion
- Lattice structure
  - space-time geometry: dimesionality& dimensions, neighbours. . .
  - point, direction: how to move on the lattice
  - field
- Algorithms
  - action
  - gauge update, gauge fixing. . .

Just respect interfaces!

Strategy of algorithms

- main structure: `LocalField<class F, int DIM>`
  - `vector<F>` ⇒ data container
  - `Geometry<DIM>` ⇒ spatial informations
  - `apply_on_timeslice<M>(M& f, const int& t)`
- `IteratorList<D>` pairs behaviour policies ∀ direction
  - `PeriodicPolicy`, `ConstPolicy`, `BulkPolicy`...

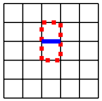
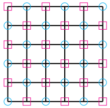
```
template <int D>
struct  TimeSliceIterList  {
  typedef  Pair<PeriodicPolicy,  typename  TimeSliceIterList<D−1>::type > type;
};
```

- `Kernel<Field_t...>` act on a single object of the field
  - void operator()(Field_t& U, const Point& n)
  - checker board hyper cube size

Parallelization

The user can choose between shared memory, distributed memory or a combination of the two

- **multithreading** via OpenMP: for each parallel kernel generate the list of points on which operate. The list is built via a checker-board scheme

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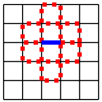

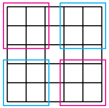

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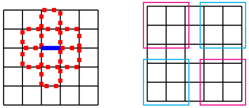
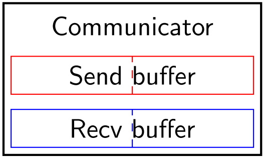
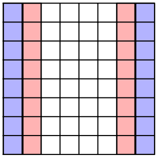
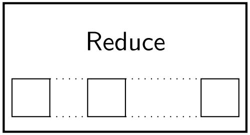


- **multiprocessing** (experimental): a `Communicator<Field_t>` contains a copy of the buffer to be sent and a recive buffer. A `Reduce<T>` performs (when required) a reduction of distributed areas.







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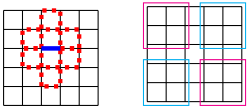

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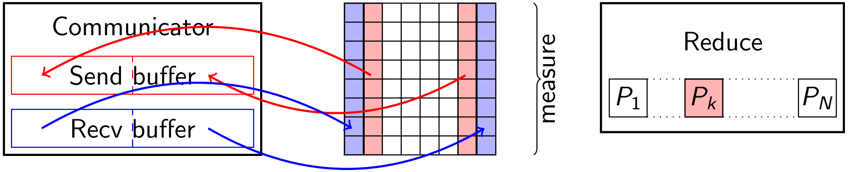
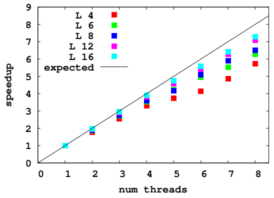
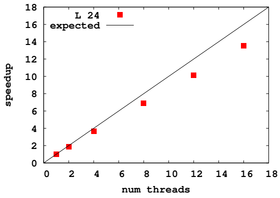


Scaling (multithread only)

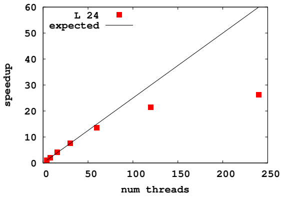
- SF regularization
- Abelian background



(a) Westmere X5680@3.33 GHz



(b) Sandybridge @2.5 GHz



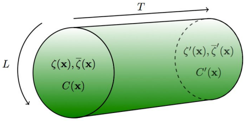
(c) Intel MIC 5110P@1.053 GHz

Multithreading look promising on different architectures, still room for improvement

NSPT for Schrodinger Functional [D.Hesse on Mon]

The boundary conditions

$$U_\mu(x + \hat{k}L) = U_\mu(x)$$
$$U_k(x)\Big|_{x_0=0} = e^{C(x)}$$
$$U_k(x)\Big|_{x_0=T} = e^{C'(x)}$$



T
L
$\zeta(\mathbf{x}), \bar{\zeta}(\mathbf{x})$
$C(\mathbf{x})$
$\zeta'(\mathbf{x}), \bar{\zeta}'(\mathbf{x})$
$C'(\mathbf{x})$

induce a background field that allows to decompose the gauge field (in PT) as

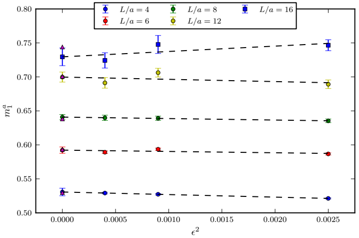
$$U_\mu(x) = \exp\{g_0 q_\mu(x)\} V_\mu(x)$$

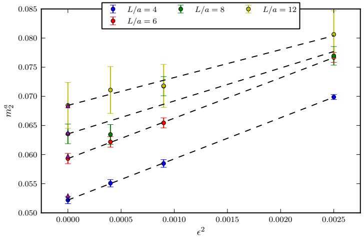
We are dealing with perturbative gluons expanded arond a nontrivial (in this case abelian) background

```
typedef bgf::AbelianBgf Bgf_t; // background field
typedef BGptSU3<Bgf_t, ORD> ptSU3; // group variables
typedef BGptGluon<Bgf_t, ORD, DIM> ptGluon; // gluon
typedef  fields::LocalField<ptGluon, DIM> GluonField;
```

One can define a coupling via

$$g^2_{SF}(L) = \frac{k}{\partial_\eta \ln \mathcal{Z}|_{\eta=0}} = g_0^2 + m_1(L/a)g_0^4 + m_2(L/a)g_0^6 + \dots$$





To give an idea of computational effort consider $L/a = 12$

$$m_2^a = 0.0684(49)$$

with a wall clock time of 210h on a single node of TCD's Lonsdale cluster (AMD Opteron, 8 cores / node)

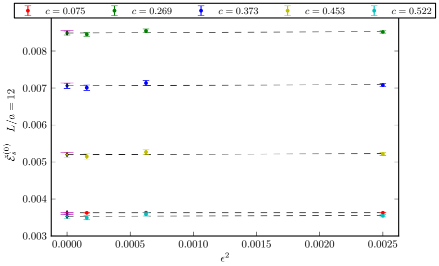
Wilson Flow D.Hesse,M.Dalla Brida [M.Dalla Brida on Mon]

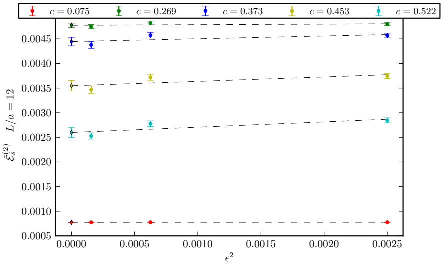
Gradient Flow on the lattice

$$\partial_t V(t)_{x\mu} = -\left\{g_0^2 \nabla_{x\mu} S_G(V(t))\right\} V(t)_{x\mu} \quad V(t)_{x\mu}|_{t=0} = U_{x\mu}$$

One can define a family of running couplings

$$\begin{aligned} \bar{g}^2_{GF}(L) &= \mathcal{N}^{-1}\langle t^2 \hat{E}(t, T/2)\rangle|_{t=c^2L^2/8} \\ &= \check{\mathcal{E}}^{(0)} g_0^2 + \check{\mathcal{E}}^{(1)} g_0^4 + \check{\mathcal{E}}^{(2)} g_0^6 + \cdots \end{aligned}$$
(*P.Fritzsch,A.Ramos*'13)





Conclusions

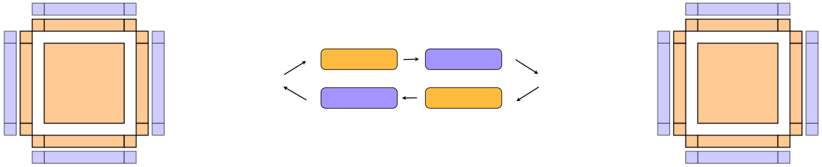
Something has been done

- ✓ periodic/SF boundary conditions
- ✓ trivial/abelian background
- ✓ Langevin gauge update algorithms: euler, 2^{nd} order RK
- ✓ Wilson flow
- ✓ multithreading

and something's on the way

- ✗ multiprocessing
- ✗ fermions
- ✗ action improvements

A strategy for the parallelization of the Wilson Dirac operator

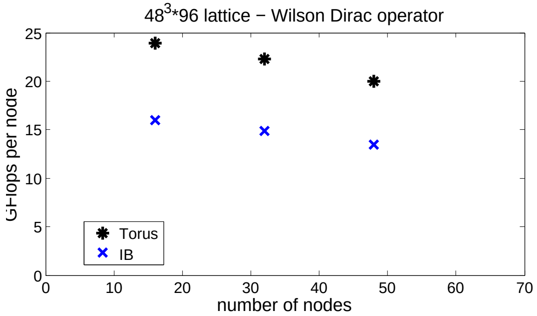


$$\psi'_{\alpha i}(x) = \sum_{\mu=1}^{4} (U_\mu^{ij}(x)(1+\gamma_\mu^{\alpha\beta})\psi_{\beta j}(x+\hat{\mu}) + U_\mu^{ij}(x-\hat{\mu})(1-\gamma_\mu^{\alpha\beta})\psi_{\beta j}(x-\hat{\mu}))$$

- Prepare borders and store them into dedicated buffers
- Half of the threads update the bulk, the remaining half exchange borders (HT: no competition on FP resources!)
- Notice that bulk is actually a bit non-trivial as a concept (one can re-allocate threads, if needed)
- Reconstruct border contributions

Results on Aurora

Wilson Dirac Operator: MPI/IB and atn/TORUS Di Renzo, Lattice2012



Peak performance percentage comparable with ETMC code on the BG/P (but with bigger node granularity).