QCDF90: Lattice QCD with Fortran 90*

I. DASGUPTA a  A.R. LEVI a  V. LUBICZ a
and C. REBBI a

aDepartment of Physics, Boston University, 590 Commonwealth Avenue, Boston,
MA 02215, USA

Abstract

We have used Fortran 90 to implement lattice QCD. We have designed a set of
machine independent modules that define fields (gauge, fermions, scalars, etc...) and
overloaded operators for all possible operations between fields, matrices and
numbers. With these modules it is very simple to write high-level efficient programs
for QCD simulations. To increase performances our modules also implements assign-
ments that do not require temporaries, and a machine independent precision
definition. We have also created a useful compression procedure for storing the
lattice configurations, and a parallel implementation of the random generators. We
have widely tested our program and modules on several parallel and single processor
supercomputers obtaining excellent performances.

1 Introduction

Simulating Quantum Chromo Dynamics (QCD) on the lattice is a challenging
task for the computers of today. The simulations involve a huge number of
variables and are so demanding on the computer resources that QCD simula-
tion is already regarded as a benchmark test for the efficiency and performance
of the modern supercomputers. With the twofold goal of facilitating the de-
velopment of algorithms and applications for lattice QCD, and of maintaining
good code performance, we have taken advantage of the possibilities offered
by Fortran 90 to write a set of modules for a high-level, yet efficient imple-
mentation of QCD simulations. Fortran 90 offers the possibility to define both

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types and overloaded operators. These two key features make Fortran 90 particularly suitable for writing QCD programs at a very high level where the algorithms are transparent and compact. On the other hand, by maximizing efficiency of the code in the definition of the overloaded operators, uniform and automatic efficiency is ensured in the entire simulation with little effort required from the high level programmer.

Our end product is a package, “QCDF90”, which is fully described in a long documentation [1], where we provide all the information needed to use our package. In the following we will highlight the main characteristics of QCDF90.

2 Precision

To render, from the beginning, the precision definitions machine independent, the module “precision” defines two kind parameters, REAL8 and LONG. These parameters store the kind of an 8-byte floating point variable and of an 8-byte integer variable.

3 Lattice geometry

The set of all lattice sites can be subdivided into “even” and “odd” sites according to whether the sum of the integer valued coordinates $x + y + z + t$ is even or odd (checkerboard subdivision). This division is actually quite useful in lattice algorithms, especially in the context of parallel implementations. In QCDF90 we implement the same checkerboarded separation of the lattice in two sublattices. Correspondingly all field variables are divided into even and odd variables. We encode this important division in the very first component of the type definitions for the fields. This component is an integer variable called parity which takes the values 0 and 1 for variables defined over even and odd sites respectively.

For the gauge variables and for the variables associated with the generators it is convenient to define a separate type for all four directions. This is realized with a second integer component variable dir which takes values from 1 to 4 for variables defined in the corresponding direction.

In a vectorized or superscalar architecture pipelined instructions and longer arrays give origin to better performance. Therefore the lattice is most efficiently indexed by a single lattice volume index ranging $xyzt$ from 0 to $NX \times NY \times NZ \times NT/2 - 1$ for each sublattices (where $Ni$ is the lattice size in direction $i$).
4 Field definitions

Here is a summary of all the types we have defined in the modules: \texttt{gauge_field} (a 3 \times 3 complex matrix in a given direction); \texttt{fermi_field} (a 3 component complex vector times 4 spinor indices); \texttt{complex_field} (a complex scalar); \texttt{real_field} (a real scalar); \texttt{generator_field} (8 real variables in a given direction, for the SU(3) generators). All the above fields are defined on an even or odd sublattice.

In addition we define the type \texttt{full_gauge_field} (a collection of 8 gauge fields) to store the entire gauge field configuration (including both parities and all directions). Moreover we defined the type \texttt{matrix} as a 3 \times 3 complex matrix.

5 Overloaded operators

To complete the high-level structure of the code one needs to define high level operators between the types described above. We define overloaded operators for all possible operations between fields, matrices, complex and real numbers. The overloaded operator set includes multiplication, multiplication with the adjoint, division, addition, subtraction, lambda matrices algebraic manipulations, gamma matrices algebraic manipulations, adjoining, conjugation, real and complex traces, exponentiation, square root, contraction, etc...

For example, if \( g_i \) are gauge fields, the use of overloaded operators allows instructions to be as simple as:

\[
g_1 = g_2 \ast g_3,
\]

specifically, such an instruction means that, at each site of the hypercubical lattice, the 3\times3 complex matrix multiplication between \( g_2 \) and \( g_3 \) is performed.

We have maximized code efficiency in the definitions of the overloaded operators. In every case, the overloaded operation is implemented with the minimum number of elementary arithmetic operations (see the section on Assignments).

Further operators have been overloaded to perform special operations involving the \( SU(3) \) \texttt{generator_fields} and \texttt{gauge_fields}. In particular it is very important to have an efficient algorithm for the matrix exponentiation, since this operation can be a time consuming component of several QCD calculations. We use a new algorithm that takes advantage of the properties of the 3 \times 3 Hermitian traceless matrices to perform the exponentiation with a minimal number of arithmetic operations.
6 Shifts and parallel transport

Shifts are also implemented as overloaded operators. For each field type C-shift implements an ordinary shift of the field with respect to the Cartesian geometry of the lattice.

Moreover, because gauge theories are characterized by the property of local gauge invariance, we find it very useful to directly define a U-shift operator that consists of the shift with the appropriate parallel transport factor. In fact in a gauge theory the parallel transport (U-shift) is the relevant shift operator and is the natural building block for programming.

The efficient manipulation of the Dirac operator is the most critical issue in QCD. For the Fermi fields we found it useful to define other shift operators which incorporate fundamental features of the Dirac operator. Firstly, one needs a shift operator that combines the naive shift with the parallel transport and the appropriate gamma matrix manipulation. This is implemented by the overloaded operators W-shift. Acting on a Fermi field $f_1$, W-shift in the direction $\mu$ produces a Fermi field $f_2$, given by

$$f_{2,x} = (1 - \gamma_\mu) U_x^\mu f_{1,x+\hat{\mu}}$$

for positive $\mu$, and

$$f_{2,x} = (1 + \gamma_\mu) U_{x-\hat{\mu}}^\dagger f_{1,x-\hat{\mu}}$$

for negative $\mu$. In these equations $U_x^\mu$ and $U_{x-\hat{\mu}}^\dagger$ are the gauge link variable necessary to implement the proper parallel transport. Combining shift with gamma matrix manipulation in the operator W-shift pays off by conserving computer resources, in fact, it follows from the properties of the gamma matrices that only one half of the spin components of the field $f_1$ undergo the transport at a time. The W-shift is the minimal specialized operator that achieves this transport.

The complete lattice Dirac-Wilson operator has been also overloaded, as well as the adjoint operator $X_{\text{dirac}} = \gamma_5 \text{Dirac} \gamma_5$.

7 Assignments

The use of overloaded operators may imply the creation of more temporaries and, consequently, more motion of data than a straightforward implementation
of operations among arrays. Consider for example the following operation among variables of type fermi_field: \( f_1 = f_1 + f_2 + f_3 \). As far as we know, Fortran 90 does not specify how the variables should be passed in function calls. As a consequence, the above instruction may require as many as four temporaries depending on the operating system. (An operating system that implements overloaded operations via function calls would first add \( f_1 \) and \( f_2 \), placing the result in a temporary \( t_1 \) whose address would then be passed to the calling program. The compiler would then copy \( t_1 \) into a temporary \( t_2 \), add \( f_3 \) to \( t_2 \) and place the result in \( t_1 \). Finally \( t_1 \) would be copied into \( f_1 \).)

The procedure could be drastically simplified and made system independent through the use of an overloaded assignment \(+=\). The above instruction could be written \( f_1 += f_2 + f_3 \) which the compiler would implement by issuing first a call to a function that adds \( f_2 \) and \( f_3 \) returning the result in \( t_1 \). The addresses of \( f_1 \) and \( t_1 \) would then be passed to a subroutine that implements the operation \( f_1 = f_1 + t_1 \) among the components of the data types. The required number of copies to memory would be only two, instead of four and it does not depend on the operating system.

In order to allow for these possible gains in efficiency, we have defined a large set of overloaded assignments. Since Fortran 90 permits only the use of the \( = \) symbol for the assignment, we have defined two global variables: a character variable assign_type and an integer variable assign_spec. The latter is introduced to accommodate assignments of a more elaborate nature. The default values of these variables are “=" and “0”. Overloaded assignments are obtained by setting the assign_type (and, if necessary, the assign_spec) to the appropriate value immediately before the assignment. Our example then becomes assign_type =’+’; \( f_1 = f_2 + f_3 \). The use of the variable assign_spec can be illustrated with another example. Consider the U-shift operation that implements shifts on gauge fields. There are in fact four U-shifts, corresponding to the four directions for the shift. To shift the gauge field \( b \) in the direction \( n \) and copy the result in the gauge field \( a \) we will use:

assign_type =’u’; assign_spec = n; a = b

Note that the assign_type and the assign_spec are automatically reset to their default values after each use. Therefore every call to an overload assignment operation must be preceded by an assignment statement. This ensure protection against misuse of the assignment.

Assignments can be defined between variables of different types. We have collected these assignments in the module “assign_mixed”. Often these assignments have very useful but not necessarily obvious definitions. For example if \( c_1 \) is a complex_field and complex is a complex variable, the instruction complex = \( c_1 \), is interpreted as setting the variable complex to the sum over all the lattice of the components of \( c_1 \).
References [1] provides a detailed explanation of all the assignment instructions.

8 Conditionals

The module “conditional” defines six overloaded relational operators, $>$, $\geq$, $<$, $\leq$, $=,$, and the \texttt{Xor} operator.

The relational operators perform two tasks: first they return a logical variable (true if \texttt{parity} and \texttt{dir} components of the operands are the same, false if they are undefined or not the same), second, and more important, they set the global variable \texttt{context} to \texttt{.TRUE.} at all sites where the relation is satisfied and to \texttt{.FALSE.} at all other sites.

The operator \texttt{Xor} admits as operands a pair of fields of the same type and returns a field, also of the same type, having as elements the corresponding elements of the first operand at the sites where the global variable \texttt{context} is \texttt{.TRUE.} and the elements of the second operand at the sites where \texttt{context} is \texttt{.FALSE.}.

This can be used to select elements out of two fields according to some local condition, an operation which lies at the foundation of stochastic simulation techniques.

9 Random numbers

We have implemented a parallelizable version of the unix pseudorandom number generator \texttt{erand48}, which also provides added functionality. \texttt{Erand48} is a congruential pseudorandom number generator based on the iterative formula

\begin{equation}
    s_{i+1} = a_1 \times s_i + b_1 \mod 2^{48},
\end{equation}

where $a_1 = 0x5DEECE66D$, $b_1 = 0xB$, $s_i$ and $s_{i+1}$ are integers of at least 48 bits of precision. The “seeds” $s_i$ are converted to real pseudorandom numbers $r_i$ with uniform distribution between 0 and 1 by $r_i = 2^{-48} s_i$.

As presented above, the algorithm is intrinsically serial. However it follows from Eq. (3) that the $N^{th}$ iterate $s_{i+N}$ is still of the form

\begin{equation}
    s_{i+N} = a_N \times s_i + b_N \mod 2^{48}
\end{equation}
with integers $a_N$ and $b_N$ which are uniquely determined by $a_1$, $b_1$. The module takes advantage of this fact and of the definitions of a global variable seeds to generate pseudorandom numbers in a parallelizable fashion. The module “random_numbers” overloads operators that generate Gaussian or uniformly distributed fields and do all the necessary seed manipulations.

10 Write and read configurations

To store and retrieve an entire SU(3) gauge field configuration, we have developed a portable, compressed ASCII format. Only the first two columns of the gauge field matrices are stored, thanks to unitarity and unimodularity. Our subroutines take advantage of the fact that all of the elements of the gauge field matrices have magnitude smaller or equal to 1 to re-express their real and imaginary parts as 48bit integers. These integers are then written in base 64, with the digits being given by the ASCII collating sequence starting from the character “0” (to avoid unwanted ASCII characters). Thus, an entire gauge field matrix is represented by 96 ASCII characters, without loss of numerical information.

To ensure the recovery of the data, a detailed description of the compressing procedure is written, as a header, at the beginning of each stored configuration file itself.

11 Performances

The code has been designed to run in any computer. It has been tested on a SGI PowerChallengeArray with 90 MHz processor nodes, using IRIX 6.1 and IRIX 6.2 and Fortran 90, with a single processor `-O3` optimization flags or with the flags `-O3` `-pfa` `-mp` to implement multiprocessing; on a Silicon Graphics Indigo using the IRIX 6.1 Fortran 90; and on the IBM R6000 58H model 7013 at 55 MHz, running AIX with the `xlf90` IBM compiler using the `-O3` optimization flags.

Memory required to execute varies according to the applications. Scales proportionally to the lattice volume $NX \times NY \times NZ \times NT$. On a $16^4$ lattice, the example codes included in QCDF90, quenched.f90 and propagator.f90 use approximately 110 Mbytes and 140 Mbytes respectively.

The run of the example programs quenched.f90 and propagator.f90 take approximately 45 microsec to update an SU(3) link, and 8 microsec to calculate
a plaquette, and 20 microsec for a CG step per link, using a $16^4$ lattice, on an SGI Power-Challenge per node.

References

[1] I. Dasgupta, A.R. Levi, V. Lubicz, and C. Rebbi, “QCDF90: A set of Fortran 90 modules for a high-level, efficient implementation of QCD simulations”, hep-lat 9605012, Comp. Phys. Comun. 98 (1996) 365 ; and reference therein.