# DEVELOPMENT IN WAVE FUNCTION METHODS MADE EASY

## WITH IRPF90 AND THE QUANTUM PACKAGE

*Anthony Scemama*, &
E. Giner, M. Caffarel, T. Applencourt, Y. Garniron
23/03/2016

Lab. Chimie et Physique Quantiques, IRSAMC, UPS/CNRS, Toulouse

# ISSUE

- Scientific codes need speed $\Longrightarrow$ : Fortran / C
- Low-level languages : difficult to maintain
- High-level features of modern Fortran (`matmul`, array syntax, derived types, ...) or C++ (objects, STL) can kill the efficiency

We need to hide the code complexity and keep the code efficient.

A simple solution : use multiple languages.

- High-level : text parsing, global code architecture, ...
- Low-level : computation
- Meta-programming : generate low-level code with a higher-level language

**Problem addressed here**

Make code in the low-level language easy to write and maintain

Programming with Implicit Reference to Parameters (IRP)

- Motivations
- The IRP method
- The IRPF90 code generator

Quantum Package

# programming with implicit reference to parameters (irp)

A program is a function of its input data:

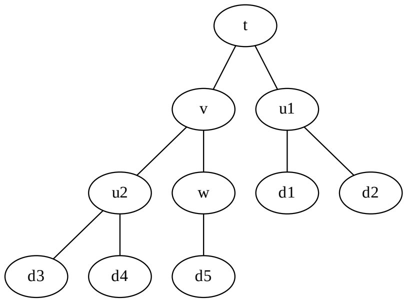
$$\text{output} = \text{program}(\text{input})$$

A program can be represented as a production tree where

- The root is the output
- The leaves are the input data
- The nodes are the intermediate variables
- The edges represent the relation needs/needed by

Example: Production tree of $t(u\,(d_1, d_2)\,, v\,(u\,(d_3, d_4)\,, w\,(d_5)))$

$$\begin{aligned} u(x,y) &= x+y+1 \\ v(x,y) &= x+y+2 \\ w(x) &= x+3 \\ t(x,y) &= x+y+4 \end{aligned}$$



# TRADITIONAL FORTRAN IMPLEMENTATION

```
program compute_t
  implicit none
  integer :: d1, d2, d3, d4 d5
  integer :: u, v, w, t

  call read_data(d1,d2,d3,d4,d5)       !            t
                                       !          /    \
  call compute_u(d3,d4,u)              !       u          v
  call compute_w(d5,w)                 !     /  |        / \
  call compute_v(u,w,v)                !  d1    d2      u    w
  call compute_u(d1,d2,u)              !              /   \    \
  call compute_t(u,v,t)                !            d3    d4    d5

  write(*,*), "t=", t
end program
```

**Imperative programming (wikipedia)**

[...] programming paradigm that uses statements that change a program's state.

- The code expresses the exploration of the production tree
- The routines have to be called in the correct order
- The values of variables are time-dependent

## Sources of complexity

1. Time-dependence of the data (*mutable data*)
2. Handling the complexity of the production tree

**Functional programming (wikipedia)**

[...] programming paradigm [...] that treats computation as the evaluation of mathematical functions and avoids changing-state and mutable data.

No time-dependence (*immutable data*) $\Longrightarrow$ reduced complexity

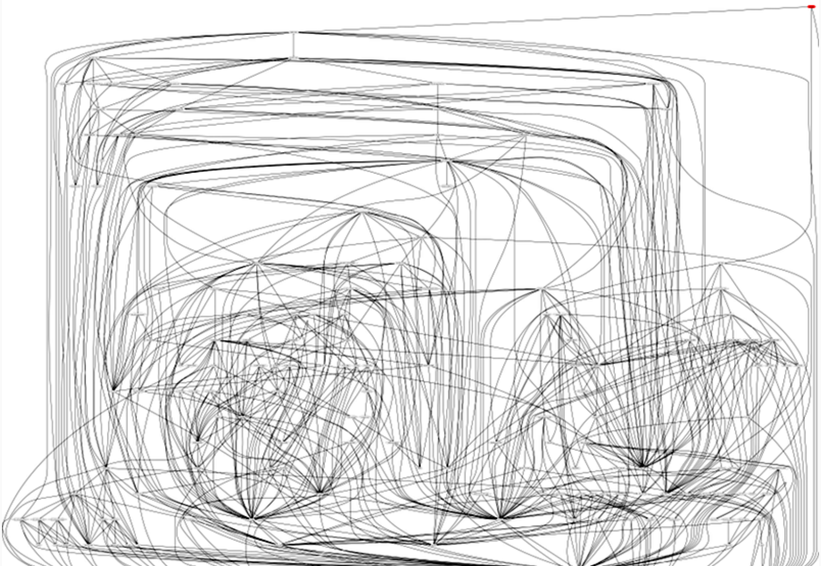
# "FUNCTIONAL" IMPLEMENTATION IN FORTRAN

```
program compute_t                      !          t
  implicit none                        !       /     \
  integer :: d1, d2, d3, d4 d5         !     u         v
  integer :: u, v, w, t                !   /   |      / \
                                       ! d1    d2    u     w
  call read_data(d1,d2,d3,d4,d5)       !           /   \    \
                                       !         d3     d4   d5
  ! Functional starts here
  write(*,*), "t=", t( u(d1,d2), v( u(d3,d4), w(d5) ) )
end program
```

- Instead of telling *what to do*, we express *what we want*
- The programmer doesn't handle the execution sequence

No time-dependence left

Production tree of Ψ in QMC=Chem: 149 nodes / 689 edges

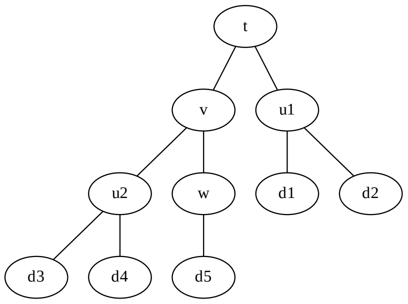


# 2. COMPLEXITY OF THE PRODUCTION TREE

1. The programmers need to have the *global knowledge* of the production tree : Production trees are usually too complex to be handled by humans
2. Programmers may not be sure that their modification did not break some other part
3. Collaborative work is difficult : any user can alter the production tree

Express the needed entities for each node:

- $t \rightarrow u_1$ and $v$
- $u_1 \rightarrow d_1$ and $d_2$
- $v \rightarrow u_2$ and $w$
- $u_2 \rightarrow d_3$ and $d_4$
- $w \rightarrow d_5$




The information is now *local* and easy to handle.

```fortran
program compute_t
  integer, external :: t
  write(*,*), "t=", t()
end program

integer function t()
  integer, external :: u1, v
  t = u1() + v() + 4
end

integer function v()
  integer, external :: u2, w
  v = u2() + w() + 2
end

integer function w()
  integer :: d1,d2,d3,d4,d5
  call read_data(d1,d2,d3,d4,d5)
  w = d5+3
end
```

```fortran
integer function f_u(x,y)
  integer, intent(in)  :: x,y
  f_u = x+y+1
end

integer function u1()
  integer :: d1,d2,d3,d4,d5
  integer, external :: f_u
  call read_data(d1,d2,d3,d4,d5)
  u1 = f_u(d1,d2)
end

integer function u2()
  integer :: d1,d2,d3,d4,d5
  integer, external :: f_u
  call read_data(d1,d2,d3,d4,d5)
  u2 = f_u(d3,d4)
end
```

# CONSEQUENCES

- The global production tree is not known by the programmer
- The program is easy to write
- Any change of dependencies will be handled properly automatically

But: The same data will be recomputed multiple times.
Simple solution : Lazy evaluation using memo functions.

Programming with Implicit Reference to Parameters (IRP)

Motivations

The IRP method

The IRPF90 code generator

**Entity** Node of the production tree

**Builder** Subroutine that builds a valid value of an entity from its dependencies

**Valid** Fully initialized with meaningful values

**Provider** Subroutine with no argument which guarantees to return a valid value of an entity

## Rules of IRP[1]

1. Each entity has only one provider
2. Before using an entity, its provider has to be called

[1] François Colonna : "IRP programming : an efficient way to reduce inter-module coupling", DOI: 10.13140/RG.2.1.3833.0406

```fortran
program test
    use entities
    implicit none
    call provide_t
    print *,  "t=", t
end program

module entities
  ! Entities
  integer :: u1, u2, v, w, t
  logical :: u1_is_built = .False.
  logical :: u2_is_built = .False.
  logical :: v_is_built  = .False.
  logical :: w_is_built  = .False.
  logical :: t_is_built  = .False.

  ! Leaves
  integer :: d1, d2, d3, d4, d5
  logical :: d_is_built  = .False.
end module
```

```fortran
subroutine provide_t
    use entities
    implicit none
    if (.not.t_is_built) then
        call provide_u1
        call provide_v
        call build_t(u1,v,t)
        t_is_built = .True.
    endif
end subroutine provide_t

subroutine build_t(x,y,result)
    implicit none
    integer, intent(in)  :: x, y
    integer, intent(out) :: result
    result = x + y + 4
end subroutine build_t
```

With the IRP method:

1. Code is easy to develop for a new developer : Adding a new feature only requires to know the *names* of the needed entities
2. If one developer changes the dependence tree, the others will not be affected : collaborative work is simple
3. Forces to write clear code : one builder builds only one thing
4. Forces to write efficient code (spatial and temporal localities are good)

But in real life:

1. A lot more typing is required
2. Programmers are lazy

Programming with Implicit Reference to Parameters (IRP)

Motivations

The IRP method

The IRPF90 code generator

- Extends Fortran with additional keywords
- Fortran code generator (source-to-source compiler)
- Writes all the mechanical IRP code

Useful features:

- Automatic Makefile generation
- Automatic Documentation
- Text editor integration
- Some Introspection
- Meta programming
- Some features targeted for HPC

http://irpf90.ups-tlse.fr

https://github.com/scemama/irpf90

https://www.gitbook.com/book/scemama/irpf90

# IRPF90 EXAMPLE

```
program irp_example
  print *, 't=', t
end

BEGIN_PROVIDER [ integer, t ]
  t = u1+v+4
END_PROVIDER

BEGIN_PROVIDER [ integer,w ]
  w = d5+3
END_PROVIDER

BEGIN_PROVIDER [ integer, v ]
  v = u2+w+2
END_PROVIDER
```

```
BEGIN_PROVIDER [ integer, u1 ]
  integer :: fu
  u1 = fu(d1,d2)
END_PROVIDER

BEGIN_PROVIDER [ integer, u2 ]
  integer :: fu
  u2 = fu(d3,d4)
END_PROVIDER

integer function fu(x,y)
  integer, intent(in) :: x,y
  fu = x+y+1
end function
```

```
BEGIN_PROVIDER [ double precision, A, (dim1, 3) ]
  ...
END_PROVIDER
```

- Allocation of IRP arrays done automatically
- Dimensioning variables can be IRP entities, provided before the memory allocation
- `FREE` keyword to force to free memory. Invalidates the entity.

```
BEGIN_PROVIDER [ double precision, Fock_matrix_beta_mo, &
                 (mo_tot_num_align,mo_tot_num) ]
 implicit none
 BEGIN_DOC
 ! Fock matrix on the MO basis
 END_DOC
 ...
END_PROVIDER

$ irpman fock_matrix_beta_mo
```

IRPF90 entities(l) fock_matrix_beta_mo IRPF90 entities(l)

Declaration

```
double precision, allocatable :: fock_matrix_beta_mo   (mo_tot_num_align,mo_tot_num)
```

Description

Fock matrix on the MO basis

File

Fock_matrix.irp.f

Needs

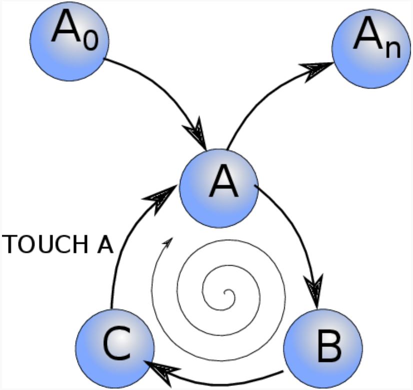
- ao_num
- fock_matrix_alpha_ao
- mo_coef
- mo_tot_num
- mo_tot_num_align

Needed by

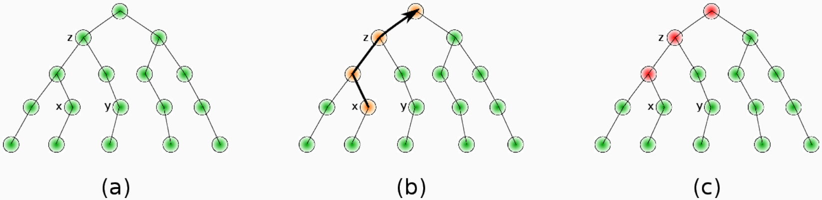
- fock_matrix_mo

MOVIE

Iterative processes involve cyclic dependencies




`TOUCH A` : `A` is valid, but everything that needs `A` is invalidated.




(a) Everything is valid

(b) *x* is modified

(c) *x* `TOUCH`ed

# MANY OTHER FEATURES

- Assert keyword, Templates
- Variables can be declared *anywhere*
- +=, −=, *= operators
- Dependencies are known by IRPF90 → Makefiles are built *automatically*
- Array alignment, Variable substitution
- Codelet generation
- TSC Profiler
- Thread safety (OpenMP)
- Syntax highlighting in Vim
- Generation of tags to navigate in the code
- No problem using external libraries (MKL, MPI, etc)
- ...

# QUANTUM PACKAGE

IRPF90 library for post-HF quantum chemistry


- Open Source (GPL) : contributors are welcome!
- Hosted on GitHub : `https://github.com/LCPQ/quantum_package`
- Goal : easy for the programmer
- Long term objective : Massively parallel post-HF

- Full-CI : $\mathcal{O}(\mathcal{N}!)$ (formally)
- CAS-CI : Full-CI in a very small space
- Complete : easy (integral $\leftrightarrow$ determinant) mapping
- Integral-driven algorithms : very efficient

**Perturbative selection (old idea re-discovered regularly)**

1. Don't explore the complete CI space, but select determinants on-the-fly (CIPSI) with perturbation theory.
2. Use PT2 to estimate the missing part

Consequences:

- Much larger spaces can be explored
- Selected : difficult (integral $\leftrightarrow$ determinant) mapping
- Determinant-driven algorithms : less efficient

**But**

The drastic reduction of the space makes the selected approach more efficient

1. Start with $|\Psi_0\rangle = |\mathrm{HF}\rangle$
2. $\forall \{|i\rangle\} \notin \Psi_n \text{ but} \in \{\mathcal{T}_{\mathrm{SD}}|\Psi_n\rangle\}$ , compute $e_i = \frac{\langle i|\mathcal{H}|\Psi_n\rangle^2}{E(\Psi_n) - \langle i|\mathcal{H}|i\rangle}$
3. if $|e_i| > \epsilon_n$, select $|i\rangle$
4. Estimated energy : $E(\Psi_n) + E(PT2)_n = E(\Psi_n) + \sum_i e_i$
5. $\Psi_{n+1} = \Psi_n + \sum_{i(\mathrm{selected})} c_i|i\rangle$
6. Minimize $E(\Psi_{n+1})$ (Davidson)
7. Choose $\epsilon_{n+1} < \epsilon_n$
8. Go to step 2

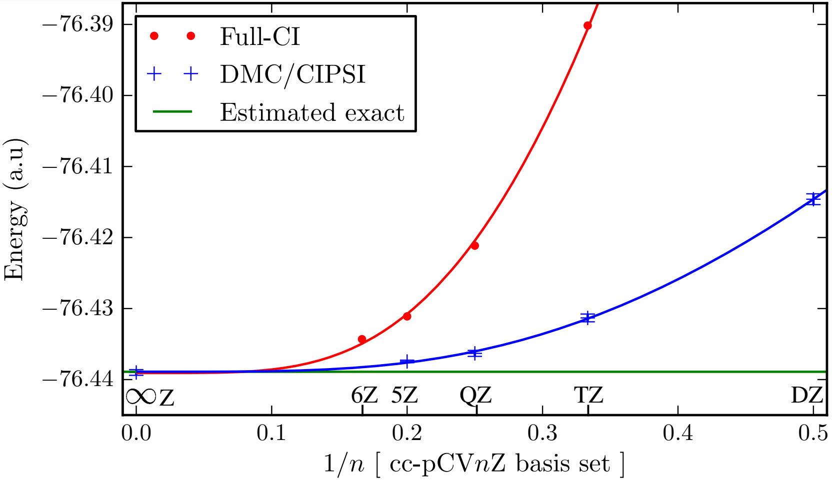
- When $n \to \infty$, $E(PT2)_{n=\infty} = 0$, so the complete CI problem is solved.
- Every CI problem can be solved by iterative perturbative selection

Perturbatively Selected CI is not a *method*, but an *algorithm*. It can be applied to

- Full-CI
- CISD, CISDT, CISTDQ, ...
- CAS-CI, MR-CI
- ...

Implies determinant-driven algorithms $\Longrightarrow$ Requires an Efficient implementation of Slater Rules

Post-Full-CI : QMC/Full-CI (E. Giner, T. Applencourt, M. Caffarel)

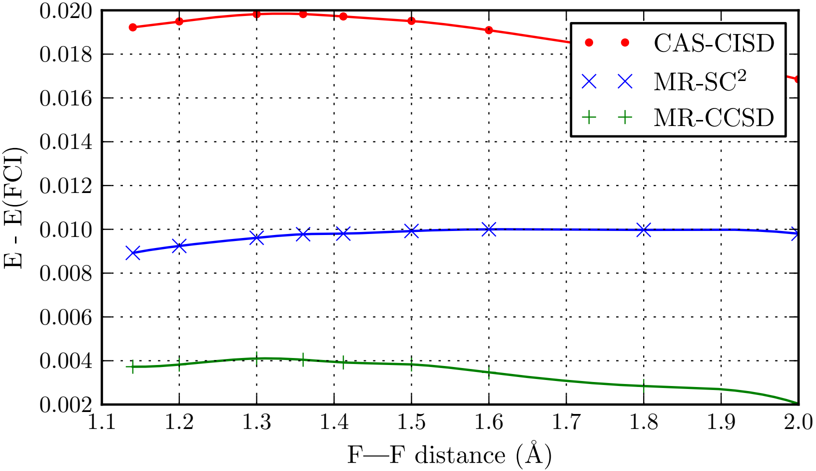


MR-CCSD : (E. Giner, G. David, J.-P. Malrieu)

TABLE VII. Symmetric dissociation of the water molecule, cc-pVDZ basis set. The FCI total energy[55] is given in $E_h$, and the deviations to this reference are given in m$E_h$. Comparison with Mukherjee's state specific MR-CC values ($E_{\text{Mk-MR-CCSD}} - E_{\text{FCI}}$) obtained from Ref. 40.

| $R$ ($R_e$) | $E_{\text{CAS-CISD}} - E_{\text{FCI}}$ | $E_{\text{Mk-MR-CCSD}} - E_{\text{FCI}}$ | $E_{\text{MR-CCSD}} - E_{\text{FCI}}$ | FCI |
|---|---|---|---|---|
| 1 $R_e$ | 4.923 | 2.909 | 1.407 | −76.241 860 |
| 1.5 $R_e$ | 4.674 | 4.817 | 1.248 | −76.072 348 |
| 2.0 $R_e$ | 3.665 | 6.485 | 0.855 | −75.951 665 |
| 2.5 $R_e$ | 3.097 | 5.672 | 0.763 | −75.917 991 |
| 3.0 $R_e$ | 2.959 | 3.987 | 0.845 | −75.911 946 |
| NPE | 1.964 | 3.576 | 0.644 | |

MR-CEPA, MR-SC$^2$ : (Y. Garniron, E. Giner, J.-P. Malrieu)
(Work in progress)



- $C_2$ Full-CI demo
- Simple Hartree-Fock