The RNPL Reference Manual

Robert Marsa
Matthew Choptuik
Center for Relativity
The University of Texas at Austin
Austin, TX, 78712-1081
marsa@hoffmann.ph.utexas.edu
matt@infeld.ph.utexas.edu

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Introduction

The acronym RNPL stands for Rapid Numerical Prototyping Language. It is a language for expressing time-dependent systems of partial differential equations and the information necessary for solving them using finite-difference techniques. It has advantages over traditional programming languages such as C and FORTRAN because it only requires the user to enter the essential structure of the program while it fills in the details.

RNPL can produce complete working programs, or a "skeleton" that the user can complete. The programs include facilities for reading parameters from a file, interactive control over output times and functions, memory management, and state dumping for calculation interruption and restart. Throughout this manual, program examples will be given in Courier, while the rest of the text will be in Times.

Program Structure

An RNPL program is completely declarative. There are no loop constructs, branch instructions, or sub-functions—just a series of declarations. These declarations can occur in any order.

The input stream is (as usual) broken up into tokens. Tokens are collections of non-white-space characters and are separated by white-space. A white-space character is a space, tab, or new-line. White-space is ignored except as a token separator, so programs are free-form in the sense of C.

1.1 Comments

There are two kinds of comments in RNPL programs. The first kind must start with a # at the beginning of a line. It continues till the end of the line. The second kind starts with // and ends at the end of the line (just like a C++ comment). The following example illustrates both kinds of comments.

```
# This is the first kind of comment
float A on grid1 // This is the second kind of comment
// So is this
```

1.2 Parameters

A parameter can be declared in several ways depending on whether it is a scalar or a vector, whether or not it has a default value, and whether or not it is a "constant." Some example declarations are:

```
parameter int fred
constant parameter float jim := 5
parameter float george[10]
parameter float ted[3] = [2.0 1.7 11]
parameter string name := "file_name"
constant parameter string comments[2] := ["comment 1" "comment 2"]
```

As the examples show, the parameter declaration begins with the reserved word parameter (optionally preceded by the reserved word constant). This is followed by a type which can be int, float, or string. Next comes a name with a size specification if the parameter is a vector. Finally, there is an optional assignment statement consisting of either = or := and a value.

Parameters provide a means of getting information to the program at run time. The use of parameters is discussed in section 4.1.

1.2.1 System Parameters

Along with the parameters discussed above, is a special type of parameter known as the system parameter. These parameters are program dependent, but must be known at compile time. Therefore, system parameters must have default values and are not read from parameter files. Currently system parameters must be scalars. There is one predefined system parameter which specifies the memory size for FORTRAN programs in doubles. Its default value is 2000000. An example statement follows:

```
system parameter int memsiz := 100000
```

System parameters are placed in a file called sys_param.inc.

1.3 Coordinate Systems

The RNPL compiler must know which names are coordinates. It further groups these names into systems. Some example coordinate declarations are:

```
rect coordinates t,x,y,z
sph coordinates t,r,theta,phi
```

First comes a coordinate system name, then the reserved word coordinates, and then a commaseparated list of names. Order is important, with the first coordinate in the list taken to be time. Any time coordinate can be repeated in other coordinate systems, but each spatial coordinate can be used only once.

1.4 Grids

Grids define the spatial regions over which the grid functions will be defined as well as their storage. A grid declaration can take one of several forms, the longest of which would be something like:

```
uniform rect[x,z] grid g1 [1:Nx][1:Nz] {xmin:xmax}{zmin:zmax}
```

The first word can be uniform or nonuniform, though only the former is currently defined. Next comes the name of the coordinate system followed by a list of coordinates on which the grid is defined. The above grid is two dimensional with coordinates x and z. After the coordinate system comes the reserved word grid followed by the grid name. Next comes the index region. In this example, the first index starts at 1 and goes to Nx, while the second starts at 1 and goes to Nz. Nx and Nz must be defined elsewhere. The index regions can contain arbitrary expressions such as [A*B+C-2:4*Nx-5/a], however, as discussed in section 2.2, it is best to keep to forms like [1:Nx] and [0:Nx-1], where Nx has been declared as a parameter. Finally, comes the coordinate region which gives the actual spatial ranges of the coordinates. In the example, we have $xmin \le x \le xmax$ and $zmin \le z \le zmax$. Coordinate regions must be of the form $\{name1:name2\}$, where name1 and name2 have been declared as parameters.

Other forms of the grid declaration leave out one or more of the above parts. The minimum allowable declaration is:

```
uniform rect grid g2
```

This declaration (along with the example coordinate declaration in section 1.3) declares g2 to be a three dimensional grid with coordinates x, y and z. The index region will be [0:Nx-1][0:Ny-1][0:Nz-1] for C output and [1:Nx][1:Ny][1:Nz] for FORTRAN output. The coordinate region will be $\{xmin:xmax\}\{ymin:ymax\}\{zmin:zmax\}$

1.5 Grid Functions

A grid function is a function defined on a grid at one or more times. Some examples of grid function declarations are:

```
float A on g1 at -1,0,1
int B on g2 at 0,1
float C on g1
float D on g2 at -1,0,1 alias
float E on g3 at 0,1 "Electric Field"
```

First comes the grid function type, either float or int. Next comes the name followed by the reserved word on and the grid name on which the function is defined. If the declaration stopped here (such as that for C above), we get a single time level. Adding the reserved word at followed by a list of offsets (positive or negative integers) gives a function defined on one time level for each offset. For instance the definition for A would give a three time level function defined at times n-1, n, and n+1. Next comes the optional reserved word alias which declares common storage for the first and last time levels. Following any of these declarations can be a string which is used as a "print name" for the grid function. Uses for the print name will be explained in chapter 2.

1.6 Attributes

An attribute is a flag array associated with the grid functions. For instance, an attribute may tell which grid functions are to be output and which are not. Attributes are defined in a similar manner to vector parameters, except the size is replaced by an encoding. The encoding is either encodeone or encodeall, with encodeone giving one value per grid function and encodeall giving one value per time level per grid function. For instance, if five grid functions are defined, three of which have three time levels each while the remaining two have two levels each, then an attribute marked as encodeone would have a length of five, while an attribute marked as encodeall would have a length of thirteen. In this case an output flag array could be defined as either

```
attribute int out_gf encodeone
or
attribute int out_gf encodeone := [0 0 1 1 0]
```

1.7 Derivative Operators

Derivative operators are operators which act on grid functions. They are used for turning differential equations into finite difference equations. Here is a declaration for a forward difference operator:

```
operator D_FW(f,r) := (<0>f[1] - <0>f[0])/dr
```

Whenever an operator is used in an expression (see section 1.12), the operator is replaced by its definition. The name f is arbitrary. It simply shows where the expression goes in the definition. For instance, if $D_FW(3*A+B,r)$ appeared in an expression, the f's in the right hand side would be replaced by 3*A+B. The notation <0>f[1] is interpreted as f_{i+1}^n , that is, f at the nth time level and i+1st grid position. The <>[] is really an operator which acts on expressions as follows:

```
<a>f[b] \rightarrow f if f is a number or parameter or time coordinate <a>f[b] \rightarrow f_{i+b} if f is a spatial coordinate <a>f[b] \rightarrow f_{i+b}^{n+a} if f is a grid function
```

Three dimensional forward difference operators would look like this:

```
operator D_FW(f,x) := (<0>f[1][0][0] - <0>f[0][0][0])/dx
operator D_FW(f,y) := (<0>f[0][1][0] - <0>f[0][0][0])/dy
operator D_FW(f,z) := (<0>f[0][0][1] - <0>f[0][0][0])/dz
```

Operator definitions can be nested as in:

```
operator D_FW(f,r) := (<0>f[1] - <0>f[0])/dr
operator D_BW(f,r) := (<0>f[0] - <0>f[-1])/dr
operator D_CN1(f,r,r) := D_BW(D_FW(<0>f[0],r),r)
operator D_CN2(f,r,r) := D_BW(D_FW(<1>f[0],r),r)
```

As you can predict, the definition of D_CN1 will result in the usual centered second derivative, namely $(f_{i+1}^n - 2f_i^n + f_{i-1}^n)/dr^2$, while the definition of D_CN2 will result in the same thing applied at the advanced time level, that is $(f_{i+1}^{n+1} - 2f_i^{n+1} + f_{i-1}^{n+1})/dr^2$. The list of coordinate names after the **f** signifies with respect to which coordinate(s) the derivative is taken.

Although operators are defined like derivatives and act as derivatives under certain circumstances (see section 1.12), they can be defined to perform other functions, such as the following definition which performs spatial averaging.

```
operator AVG(f,r) := (<0>f[1] + <0>f[0])/2
```

Because operators are internally treated as derivatives, even definitions such as this need the coordinate list.

1.8 Residuals

Residuals define the system of equations, typically by using derivative operators. Consider the following residual definition:

Assuming the proper definitions of the derivative operators, this residual will encodes the linear wave equation on a string with the end points fixed. An equivalent declaration would be:

First comes the reserved word residual followed by the name of the grid function whose residual is being defined. Next comes a bracket-enclosed set of index regions and expressions. The index region shows over what range the expression is a valid description of the behavior of the system.

The union of the index regions should equal the index region of the grid on which the function is defined, but this is not required. Note that each region-expression pair is separated by a semi-colon.

The residual tells how to determine the advanced value of a grid function. Thus, the residual must contain <a>f... where a is the offset to the most advanced time level defined for grid function f

Part of a residual for a three dimensional grid function would look like:

```
residual A { [1:Nx][1:1][1:1] := D_LF(A,x) + D_FW(B,y) ;

[Nx:Nx][1:Ny][1:Nz] := <1>A[0][0][0] = 5.0*C }
```

The reserved word residual can be preceded by the reserved word evaluate which tells the compiler to produce code which will evaluate the residual.

In addition, the word residual can be followed by a global offset for example:

```
residual <1>[0] A { [1:Nx] := ... }
```

This offset is applied globally to each expression appearing in the residual. See section 1.12 for more information on expressions.

1.9 Initializations

An initialization defines the initial data for a grid function. Its form is identical to the residual declaration with residual replaced by initialize. However the expression is interpreted differently. Consider the following initialization declaration:

```
initialize phi { [1:Nr] := amp*exp(-((r-c)/delta)^2) }
```

Unlike the residual declaration, the expression in the initialization must not contain its grid function. The retarded time level of the grid function is set to the expression. In the case above, phi will be set to a Gaussian.

1.10 Loop Driver

The loop driver declaration has the form looper name, where name is any identifier. When the compiler processes the driver statement, it looks in its library directory for a file called name.drv_lang, where lang is c, f77, or f90. It then simply includes this file into the generated source.

There are currently two predefined loopers: iterative and standard. The iterative looper makes an initial guess at the advanced grid function values, then calls the update routines and iterates until the norm of the residual is below a threshold. The standard driver just calls the update routines.

1.11 Updates

Update declarations can take many forms. Here are some examples:

```
auto update phi,pi,beta
stub evolver updates A.B.C
```

```
header A, B[Bnp1,Bn,Bnm1], C[C], x,y,z,dt,auto work#0(5*Nx*Ny*Nz), static work#1(3*Nx*Ny-.5*Nz)
```

myroutine.inc myupdate update A,B header A,B,dt

The first form defines an automatic update. The declaration above would cause the compiler to produce a routine to update the grid functions phi, pi, and beta if residuals have been declared for them. Otherwise, the compiler has no idea how to update the grid functions and will produce an error message.

The second declaration will cause the compiler to produce the header for a routine called evolver which is expected to update grid functions A, B, and C. The body of the routine is left blank, to be filled in by the user. Following the reserved word header, comes a list of things to appear in the calling sequence for the function. A grid function name such as A above will cause all the time levels of A to be passed to the function. If A has three time levels (1,0,-1), then they will be named A_np1, A_n, and A_nm1 by default. The user can provide his own names to override the defaults as in the case of B. If only one name is provided (as for C), the time levels will be passed in as the elements of a single vector, the first component of which will be the advanced time level.

Other things that can appear in the header list are coordinates (such as x,y,z above) and coordinate differentials (such as dt). Parameters can also be included in the list. Work arrays are declared like the final two parameters. First comes auto or static. Static work arrays are declared at the start of the program and persist throughout. Auto work arrays are allocated before the call to the update routine and are destroyed afterwards. Next comes the word work followed by the # symbol and an integer. This integer is tacked onto the end of the word work to form the name of the array. Finally comes an expression for the size of the work array enclosed in parentheses.

1.12 Expressions

Expressions are made up mainly of identifiers separated by operators. RNPL defines the usual set of arithmetic operators (+,-,*,/) along with exponentiation (^ or **). The operators obey the usual precedence rules.

Identifiers may be names of grid functions, coordinates, or parameters. In addition, grid functions may be supplied with temporal and spatial offsets (see section 1.7), and coordinates may be supplied with a spatial offset.

Expressions can also contain the well-known functions exp, log, tan, sin, cos, sinh, cosh, tanh, and sqrt as well as derivative operators.

Here is an example of a complicated RNPL expression:

```
a*b+(c*2.67/<0)phi[1] + d^2/tan(theta) - r[-1]*D_(phi*3/a,r) + cos(3*eta)*D_(eta+D_(phi,r),r) + expand D_(a*b + c,r)
```

You'll notice the word expand before the last derivative operator. This tells RNPL to symbolically expand the derivative before making the operator substitution. Thus, the final term is equivalent to:

```
D_{(a,r)*b} + a*D_{(b,r)} + D_{(c,r)}
```

Implementation

2.1 Case Sensitivity

Identifiers in RNPL are case sensitive if the target language is C and are case insensitive if the target language is FORTRAN. Regardless of the target language, reserved words may be given in all lower case or all upper case. Case combinations will produce syntax errors.

2.2 Coordinate Differentials

Coordinate differentials are assumed to be anything that is a coordinate name with a d in front of it, such as dt or dx if t and x are coordinates. A coordinate differential is defined by the index region and coordinate region of the first grid which uses its coordinate. For instance, if the following coordinate system and grids are defined:

```
rect coordinates t,x,y
uniform rect grid g1 [1:Nx][1:Ny] {xmin:xmax} {ymin:ymax}
uniform rect[x] grid g2 [1:N] {min:max}
```

then dx will be defined from g1 by dx = (xmax - xmin)/(Nx - 1) even though g2 may have a different coordinate spacing.

2.3 Special Parameters and Attributes

There are several "special" parameters defined by RNPLThese are declared by the program (if not by the user) and given default values. They will be read from the parameter file if it contains them. These parameters are shown in the following list along with their definitions and default values.

```
constant parameter float start_t := 0 // start time
constant parameter int iter := 100 // number of iterations
constant parameter float epsiter := 1e-5 // iteration threshold
constant parameter int fout := 0 // file output (0 no, 1 yes)
constant parameter int ser := 0 // fs output (0 no, 1 yes) if appropriate
constant parameter float lambda := .5 // dt/dr, dr=sqrt((dx^2+dy^2+dz^2)/3)
constant parameter int rmod := 1 // output every rmodth time step
```

The names N<c>, where <c> is a coordinate, are declared internally to RNPL. They are NOT parameters, nor should they be declared by the user. N<c> is defined at run time by N<c> = N<c>0 $2^{level}+1$. Thus, if a grid is defined with an index region of length N<c>, it will be automatically scaled simply by changing the value of level in the parameter file. Grids defined in this way will always have an odd number of points in each dimension.

There is one pre-defined attribute: out_gf. This is an integer array with one element for each grid function, that is:

attribute int out_gf encodeone

Each element is assigned the default value of 0. This element tells whether output is enabled for that grid function or not. The values of this attribute can be changed during program execution.

Compiler Usage

3.1 Code Generation

The RNPL compiler is called from the command line with the following command:

rnpl -lang [program_file]

The switch -lang tells RNPL what the target output language is, c, f77, or f90.

The compiler generates code for two programs, the solver and the initial data generator. If program_file is specified, rnpl will output the solver code to a file. The extensions .rnpl or _rnpl will be removed from the end of program_file if they exist. The appropriate extension for the output language is then appended (.c or .f). The initial data generator is written to program_file_init plus the appropriate extension (.c or .f) If no program_file is specified, rnpl reads from stdin and writes to stdout. In this case, the initial data generator goes to r_out_init (.c or .f). Errors are directed to stderr.

RNPL sends the code for the update routines to a file named updates (.h or .f). Also, a default attribute file is produced, named .rnpl.attributes.

In the case of FORTRAN output, two include files named globals.inc and other_glbs.inc are also produced.

The compiler needs certain support files which it looks for in the current directory or in the directory defined by the environment variable RNPL_PATH.

3.2 Target Language Compilation

Once the RNPL compiler has been executed, the C or FORTRAN sources must be built. In the case of C output, simply compile the two .c files since updates.h is automatically included. For FORTRAN code, compile the solver and updates.f and link them together.

Generated Programs

4.1 Parameter Files

A parameter file is an ASCII file containing arbitrary text along with lines of the form name := value, where name is the name of a parameter, and value is its new value. At run time, RNPL generated programs will read this file and use any values found to initialize parameters.

Here is an example parameter file:

```
This is a parameter file
tag := "a_"
level := 1
Nx0 := 100
xmin := -10
in_file := "init_data.hdf"
out_file := "dump.hdf"
```

4.2 Solver

If RNPL is run on wave.rnpl and the resulting source files are then compiled into executables named wave and wave_init, then the solver (wave) can be executed by typing "wave param_file" or "wave" on the command line. Param_file is an ASCII file of parameter values as discussed above. If no parameter file is given on the command line, the program will prompt for one. If there is no initial data file (in_file), wave will execute wave_init to generate one. If wave_init doesn't exist, wave will print a warning and continue without reading the initial data. If there is an initial data file, wave will read it and continue. Every rmod time steps (rmod is a parameter), wave will generate output as specified by out_gf, ser, and fout. It will print the current step and value of time to stdout. During execution, the user can type \hat{C} or \hat{Z} to stop wave. A menu will then be presented which allows the user to change the output frequency (rmod) and which grid functions will be output (out_gf). The user can also choose to quit. Upon termination (either forced or after "iter" time steps), wave will dump state to out_file. Execution can later be resumed by copying out_file to in_file and rerunning wave.

4.3 Initial Data Generator

The initial data generator can be run from the command line as well as being called by the solver. It reads the same parameter file as the solver and writes the initial data to in_file.

4.4 Output

One of the design goals of RNPL is to provide uniform and automatic access to I/O facilities to aid the user in examining the results of computations. As discussed in section 2.3, there is currently one pre-defined attribute: out_gf. If the special parameter fout is set, then every rmod time steps, output is generated for every grid function for which output has been enabled via out_gf. Output is to .hdf files: one file for each selected grid function is created, and each file consists of a sequence of dumps labelled with the actual output time. These files can then be post-processed with a variety of software, including the ExplorerTM module, ReadHDF_GFTO available via anonymous ftp from helmholtz.ph.utexas.edu in /pub/explorer/modules.

The interface to the lower level .hdf routines is also directly accessible from C or Fortran codes which have *not* been generated using RNPL and is described in *The RNPL User's Guide*.

RNPL Grammar in BNR Format

$\operatorname{dec_list}$	\rightarrow	
		dec_list declaration
declaration		param_dec coord_dec grid_dec gfunc_dec attrib_dec d_operator residual initialization looper update
param_dec	→ 	param p_type name param p_type name assignop scalar param p_type name v_size param p_type name v_size assignop vector const param p_type name const param p_type name assignop scalar const param p_type name v_size const param p_type name v_size const param p_type name v_size
$\operatorname{coord} \underline{\operatorname{dec}}$	\rightarrow	name coordinates coord_list
grid_dec	→ 	g_type name grid name i_region c_region g_type name grid name g_type name obrack coord_list cbrack grid name i_region c_region g_type name obrack coord_list cbrack grid name
gfunc_dec	→ 	type name on name type name on name str type name on name at o_list

		type name on name at o_list alias type name on name at o_list str type name on name at o_list alias str
attrib_dec	\rightarrow	attrib p_type name encoding assignop vector
$d_operator$	\rightarrow	operator d_op assignop expr
residual	→ 	resid name obrace res_list cbrace resid time index name obrace res_list cbrace evaluate resid name obrace res_list cbrace evaluate resid time index name obrace res_list cbrace
initialization	\rightarrow	initialize name obrace res_list cbrace
looper	\rightarrow	looper name
${f update}$	→ 	name name update coord_list header ref_list stub name update coord_list header ref_list auto update coord_list
p_type	→ 	int float string
name	\rightarrow	iden
scalar	→ 	inum minus inum num minus num str
v_size	\rightarrow	obrack inum cbrack
vector	\rightarrow	obrack scalar_list cbrack
coord_list	$\stackrel{\longrightarrow}{\mid}$	name coord_list comma name
g_type	→ 	uniform nonuniform
i_region	\rightarrow	obrack expr colon expr cbrack obrack expr colon expr cbrack i_region
c_region	\rightarrow	obrace name colon name cbrace

		obrace name colon name cbrace c_region
type	$\overset{\longrightarrow}{\mid}$	int float
o_list	→ 	inum minus inum o_list comma inum o_list comma minus inum
encoding	\rightarrow	encodeone encodeall
d _ op		name oparen expr comma coord_list cparen expand name oparen expr comma coord_list cparen
expr		expr plus expr expr minus expr expr equals expr expr times expr expr divide expr expr caret expr plus expr minus expr oparen expr cparen d_op func gfunc coord name num inum
res_list	\rightarrow	i_region assignop expr res_list scolon i_region assignop expr
time	→	oabr inum cabr oabr minus inum cabr
index	→ 	obrack inum cbrack obrack minus inum cbrack obrack inum cbrack index obrack minus inum cbrack index
ref_list	\rightarrow	reference ref_list comma reference
scalar_list	\rightarrow	scalar

Terminals

encodeall

parameter or PARAMETER param assignop := or =coordinates coordinates or COORDINATES grid grid or GRID obrack cbrack on or ON on \mathbf{at} at or AT attrib attribute or ATTRIBUTE operator operator or OPERATOR residual or RESIDUAL resid obrace cbrace evaluate or EVALUATE evaluate initialize or INITIALIZE initialize looper looper or LOOPER update or updates or UPDATE or UPDATES update int int or INT float or FLOAT float string string or STRING iden see below inum positive integer minus num positive real number \mathbf{str} "any characters" comma uniform or UNIFORM uniform nonuniform or NONUNIFORM nonuniform colon encodeone or ENCODEONE encodeone

encodeall or ENCODEALL

```
oparen (
cparen )
expand expand or EXPAND
plus +
times *
divide /
caret ^ or **
scolon ;
oabr <
cabr >
```

An iden is string which starts with a letter or _ and contains letters, digits, and _. It can also be two or more iden's separated by . or ->. For example, the following are valid iden's:

frank
AlBerT0
_george123fred__
brad.charles

employer->name.first

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Bibliography