Introduction to mn-fysrp-pic

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1 Introduction

The mn-fysrp-pic Git repository holds the official Particle-In-Cell (PIC) code belonging to the 4Dspace project and the Plasma and Space Physics group at the Physics Department of UiO. In order to keep the PIC code and their different versions clean and manageable and to avoid conflicts during cooperation it is of utmost importance that all users obey the rules of the repository. Each user is therefore responsible of making himself/herself familiar with the rules stated herein. Failure to do so may result in reduced privileges in the repository.

2 Workflow

The mn-fysrp-pic repository utilizes what's called a Feature Branch Workflow¹ as illustrated in Fig. 1. The reason for this is to allow several users to develop functions for the code independently with a minimum of conflicts. It also assures that a fully functioning version of the code is always accessible. Using Git also means that all previous revisions of the code are retrievable. This, along with information on which revision was used to generate a set of results, make the experiments reproducible.

To briefly explain the Feature Branch Workflow, the master branch should always represent a fully functional version of the PIC code. Whenever a new feature is to be developed a new feature branch (e.g. Feature 1 in the figure) is created and the user works on that branch until the feature is finished. Then, it is merged back onto the master branch. The user verifies that the master branch executes and is fully functioning before pushing the changes to the central repository (the origin). Ruining the central master branch causes trouble for other users who expect it to be up and running.

Let's consider an example: One user starts implementing a new input settings system for the PIC code (Feature 2). At the same time another user starts revising the field solver (Feature 3). Each user can make as many commits as desirable within their feature branch for the sake of backup. The input system is finished first and its feature branch is merged back onto the master branch before being deleted. It doesn't matter that another user has edited parts of the field solver because that's in another branch. The master branch is now a fully functional PIC code with new input system but with the old solver left intact. Once the new solver is finished, it is merged back to the master. But the master has changed since the revision Feature 3 is built upon. These changes, however, most likely affect other files and Git will be able to seamlessly merge only the appropriate lines changed during Feature 3 development. If uncertainties occur, Git will ask the Feature 3 developer to do some manual work to properly merge Feature 3 with the master branch. Feature 2 will not be overwritten.

Feature branches normally only exist locally. If desirable, they can be pushed to the central repository (the origin) to make them accessible from several computers (for instance for collaboration). The origin should be kept clean, however, meaning that someone must be responsible to delete the branches after merging ensuring that only a few branches exist centrally. Only the repository administrator has the privilege to delete branches and cleaning the origin so other users

 $^{$^{-1}$}See more about various Git workflows here:$ <code>https://www.atlassian.com/git/tutorials/comparing-workflows</code> .

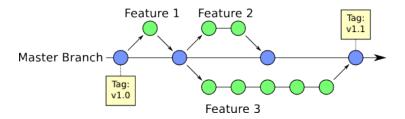


Figure 1: Illustration of Feature Branch Workflow

should ask for permission before pushing new branches to the origin. Moreover, the branches pushed to origin should have globally understandable names.

Finally, some revisions can be tagged with a version number, making it easier in publications to refer to a specific revision of the code. This should only be done with revisions on the master branch.

As a summary: feature branches can have many revisions allowing the developer to go back in case of mistakes, for backup, and for sharing code with other developers. The master branch is holy and only fully functional features should be merged into it.

If this section is unclear and more advice on Git is needed please refer to mn-fysrp-pic/docs/git.pdf before making any changes to the repository.

3 Setting up a Local Copy

To access the repository and be able to make changes you need to set up a local copy. To get access you need an SSH key-pair (public and private keys). Unless you already have that you can run the following command²:

```
ssh-keygen -t rsa -b 4096
```

This generates the following files:

• Private key: ~/.ssh/id_rsa

• Public key: ~/.ssh/id_rsa.pub

The private key is private (hence the name) and should under no circumstance be shared with others. It is what you use to authorize when logging into the remote server. The public key cannot be used to log in but is used by the remote server(s) to verify that you have the private key.

Rename a copy of your public key to <username>.pub where <username> is your UiO username, and mail it to the repository administrator (sigvaldm@fys.uio.no) and wait for approval.

Next, configure your local git user using these commands:

```
git config --global user.name '<username>'
git config --global user.email '<email>'
```

Go to the folder where you'd like your local copy (typically your home directory), and clone the central repository (origin) like this:

²http://www.uio.no/tjenester/it/maskin/filer/versjonskontroll/git.html .

```
git clone gitolite@git.uio.no:mn-fysrp-pic
```

A new folder with the name mn-fysrp-pic will be created. This is your local working copy.

If you want access from another computer (e.g. supercomputer) you have to copy your private key to ~/.ssh/id_rsa on that computer, and run the configuration and cloning steps there as well.

4 Repository Structure

4.1 Folder Structure

The mn-fysrp-pic repository has the following folder structure (unimportant details omitted):

```
mn-fysrp-pic/

doc/

doxygen/
html/(gitignored)
introduction/
latex/(gitignored)
introduction.pdf
lib/
old/
proof of concept/
src/
input.ini
makefile
pinc (gitignored)
```

doc contains documentation of the code and the repository. That includes this document (introduction.pdf) along with a similarly named folder containing the LATEX source files used to create it. html and latex contains documentation of the code in HTML and LaTeX, respectively. This documentation is not, strictly speaking, part of the repository, but rather is auto-generated by Doxygen from the files in the repository when building the code. The doxygen-folder includes auxiliary files needed by Doxygen to do this.

Small non-standard third party libraries are shipped with the code for convenience. They are put under the folder lib uncompressed but otherwise as provided by the manufacturer, i.e. uncompiled and with legal information files/licenses. Unfortunately, it has too many drawbacks to include big standard libraries in this folder and perform static linking even though this would've guaranteed consistent executions across computers. See Sec. 5.

The source code is located at src and it is the primary task of the repository is to act as a Version Control System (VCS) for the code (.c-files and .h-files) within this folder. The repository should not track object (.o) files, compiled and

Table 1: Source file categorization

	.c-files	.h-files			
Main routine	main.c				
Framework	aux.c	pinc.h			
	grid.c				
	io.c				
	population.c				
Multigrid module	multigrid.c	multigrid.h			
Future module	moduleA.c	module.h			
	moduleB.c				

linked executables, binaries or similar (also true for third party libraries). VCSs like Git only needs to keep track of the lines changed in text files which makes them very efficient. Other files such as executables and object files carry no real information to the programmer and must be re-stored in entirety every time it changes (after each compilation). Many such files can make the repository heavy. It also clutters the repository with unnecessary changes each time someone recompiles the whole program, causing unnecessary Git conflicts. For this reason these file types are added to .gitignore which means that they will not be committed to the repository.

The folder proof of concept may be used to test smaller pieces of code, for instance to check the fastest way to implement something. If, for instance, it was found that one way of implementing something is faster than the other, it might be desirable to keep this experiment for future evidence. This folder is *not* intended to store lots of old rubbish, it should exclusively be something that is clean enough to re-open and and (with little effort) refer to. The folder old may temporarily hold old files which are to be deleted once a replacement is developed.

Finally, simulation .h5-files should not be part of the repository. They are incredibly large and there is also no reason to have version control on them; once a simulation is successfully run, and maybe even used in publications, it should be considered static. Simulations and their input files are also not, strictly speaking, part of the program.

4.2 File Structure

The PINC source files can be thought to belong to one of three categories as illustrated in Tab. 1:

main.c is the main-routine, whereas pinc.h is the main header file declaring a framework for all PINC modules (pedantically it's not a framework but is thought of as such). It declares datatypes and functions for handling particles and grid quantities along with functions to manipulate them and other building block functions ensuring a coherent code. The definitions are stored in the accompanying .c-files. Modules, for instance a multigrid solver, is implemented in a .h-file and one or more .c-files starting with the name of the module. The framework files should not depend on the modules.

5 Compiling and Running PINC

Before being able to compile PINC the following libraries must be installed:

- 1. OpenMPI
- 2. GNU Scientific Library (GSL)
- 3. HDF5 API including parallel support (more on parallel support later)

These are typically installed either through sudo apt-get install when available or by downloading the source code and executing something like this:

```
./configure
make
sudo make install
```

The last step is crucial since this makes the system find the library without having to add local modifications to the PINC makefile. While it is permitted to do whatever you like locally, it is not permitted to push files of local relevance only to origin, and it is therefore advised to install the libraries on the system.

Once dependencies are resolved PINC is compiled using the makefile in the repository:

```
cd mn-fysrp-pic
make
```

The makefile installs the libraries in lib as well as generating Doxygen documentation. When adding new header or source files these can be added to HEAD_ or SRC_, respectively, in the makefile. Next, PINC is executed as

```
./pinc input.ini
```

or for more than one processes (2 in this example):

```
mpirun -np 2 pinc input.ini
```

input.ini is a template input file for PINC. To erase all build files run

```
make clean
```

6 Coding Practices

6.1 Naming Conventions

We use the camelCase-convention rather than underscore. E.g.

```
1 | int myVariable = 0;
2 | void myFunction();
```

Names should be intuitive rather than short. On the other hand, too long names are bothersome too. Obvious abbreviations are okay. Common abbreviations and names are okay too even if hard to read simply because their commonness makes them more likely to be understood than easier but unfamiliar names. Examples:

- knErg is a worse name than kineticEnergy which is a worse name than energy (if kinetic energy is the only kind of energy that makes sense).
- wij1k1 is a horrible name.
- temp is a perfectly understandable name for a temporary variable inside a sufficiently short scope. No need to call it kineticEnergyFromPreviousTimeStep . temp2 however is usually a sign that you need to clean up.
- i and j are perfect names for a loop counters. No need to call it loopCounter. Make sure to avoid confusion with common uses of i and j in PINC, though.
- argc and argv are okay since they are understood by any C programmer.
- pos is okay since it's obviously a contraction of "position".

Generally speaking, the larger the scope a variable or function has the more important is its proper naming.

6.1.1 Grammar

Moreover we have the following grammar conventions:

- nelements. "n" in the beginning of a variable name like this is read like "the number of". The word(s) that come after "n" should be plural. You don't say "the number of element".
- In many cases it is a good idea that arrays have plural names. Consider this example:

• Because of the above point, datatypes (and structs) should have singular names. Consider these examples

6.1.2 Structs

Structs are named with a capital first letter to indicate that it is a struct:

```
1 | typedef struct{
2 | ...
3 |} MyStruct;
```

Table 2: Suggested names in PINC

	С	Math
time step	n	n
number of time steps	nTimeSteps	N_t
dimension	d	d
number of dimensions	nDims	N_d
specie	S	s
number of species	nSpecies	N_s
particle index	i	i
number of particles		N_p
node index within local MPI subdomain	p=func(j,k,1)	p = f(j, k, l)
MPI node index	P=func(J,K,L)	P = f(J, K, L)
node index in global grid	<pre>gp=func(gj,gk,gl)</pre>	p' = f(j', k', l')

More precisely, we actually do *not* give the struct a name, but rather name its datatype using typedef. Naming the struct would look something like this:

Naming both the struct and the datatype means that the same variable could be declared using two notations and we strive for consistency:

```
1 | MyStruct newInstance; // CORRECT 2 | struct MyStruct newInstance; // WRONG
```

The only exception I can think of when naming the struct itself is necessary is when using opaque datatypes, if that will ever be relevant.

6.1.3 Indices

In numerical codes there are often many indices. As an effort to avoid confusion one should not use one variable name for loop counter of particles one place and for grid another place. Tab. 2 shows names which are to be used for loops through grids or particles along with comparisons to how they could be written mathematically.

Consider for instance iterating through all species:

The grid quantities are stored in a flat manner in one-dimensional arrays. Thus a conversion between three-dimensional indices (e.g. (j, k, l)) and a flat index (e.g. p) is required. The table lists both flat and three-dimensional indices.

If nested loops need to iterate across the same index simply use a double letter for the inner loop (e.g. ii for particles or gjj for global grid).

In functions not dealing with particle or grid quantities it is perfectly valid to use e.g. i or j as loop counters for generic purposes. Please also see the documentation of the <code>Grid</code> and <code>Population</code> structs to get a better understanding of naming conventions.

6.2 Program Structure

- No global variables allowed.
- Globally available functions of course must be declared in .h-file. Functions which are only used locally within one translation unit (one .c-file) should be declared in the top of that file before any function definitions (mind the difference between declaration and definition). Local functions should also be defined static. inline can be used the way it is intended but should not be exaggerated and only works on local functions!
- Do not copy large chunks of data unnecessarily, i.e. by passing structs to functions. The preferred way is to initialize data at one place and rather pass along the address (either through call-by-reference or through pointers).
- Brackets do not get separate lines. Correct:

Wrong:

- The code should compile without any errors or warnings. Tweaking compiler options in makefile just to achieve this is not permitted.
- Whenever a function takes in a pointer to a variable that is not to be modified (e.g. a string) it should be declared const:

```
1 | void function(const char *str);
```

This serves two purposes: (1) it prevents accidentally changing the content of the variable inside the function. (2) It tells other developers that this

function will not change the content of this variable. If a local copy is to be made inside the function it needs to be recast to allow editing:

```
1 | char *temp = (char*) str;
```

- Many numerical codes output way too much information to terminal. Computed auxiliary values generally should not be output to terminal but to file. Only messages on progression status, warnings and errors belong to the terminal. Use the PINC-specific command <code>msg()</code> to do this rather than <code>printf()</code> in order to ensure a consistent output behaviour. Auxiliary variables and more extensive messages can be printed to file using <code>fMsg()</code>. See documentation of <code>msg()</code> and <code>fMsg()</code>.
- Do not make new datatypes hiding pointers. Counter-example:

```
1 | typedef double* doubleArr; // WRONG
```

This hides what is actually going on and therefore makes it more difficult for other programmers to understand. C-programmers need to be confident about their pointers. The only permitted exception is opaque datatypes (if that is ever needed).

6.3 Comments and Documentation

• Multi-line comments should be written the following way:

```
1 | /*
2 | * This is my comment.
3 | * This is also my comment.
```

• If desirable, the document can be organized using sections and titles. Sections and titles look like this:

The last character on the section comment should be on column 80.

• Doxygen is used to auto-generate documentation of the code. Doxygen comments are written the following way (note the extra * on the first line):

Each file starts with a Doxygen-comment looking something like this:

```
2
    * Ofile
                            main.c
3
    * @author
                            Siguald Marholm <sigualdm@fys.uio.no>
4
      @copyright
                            University of Oslo, Norway
5
    * @brief
                            PINC main routine.
6
                            11.10.15
8
     More extensive description
```

All functions are documented by a Doxygen-comment looking something like this just in front of the function declaration. Example:

```
2
   * Obrief Brief one-line description of function
3
    * @param
                   in
                           Integer in.
    * @param[out]
                            Result is stored in this variable.
4
                   out.
5
     @return
                   void
     More extensive description.
7
  void function(int in, int *out);
```

• As a rule of thumb: Comment what functions does, not how. If "how" needs exhaustive explanation probably the function should be rewritten. "What" should be documented in the Doxygen comment.

6.4 Formatting and language

- English is the working language.
- Use tab for indentation, not spaces. One tab should be set equal to 4 spaces.

- Output printed to terminal should be no more than 80 columns/characters as this is the default terminal width.
- Lines in source files should be no longer than 132 columns/characters, although doxygen comments should stop at column 80.
- Whenever a date is to be written, for instance in a Doxygen comment, it is written dd.mm.yy.
- Try to avoid incomplete sentences and poor language in comments, especially in Doxygen comments. End sentences with period.

7 Tools

7.1 Valgrind

To ensure that dynamically allocated memory is freed use Valgrind. Since Open-MPI generates a lot of false positives these false positives are suppressed by using the PINC wrapper script valgrind.sh for running Valgrind instead of just valgrind³. First, make sure valgrind is installed on your system. Then, consider the following example:

```
void test(){
            char *ptr = malloc(1048576);
2
3
4
5
   int main(int argc, char *argv[]){
6
            char *str = malloc(16);
7
8
            strcpy(str,"test");
9
10
            test();
11
12
            printf("%s\n",str);
13
            return 0;
  1}
14
```

Then, compiling and running valgrind as follows:

```
make clean
make COPT=
   ./valgrind.sh ./pinc input.ini
```

returns (uninteresting details removed):

HEAP SUMMARY:

```
in use at exit: 1,255,872 bytes in 498 blocks total heap usage: 7,251 allocs, 6,753 frees, 14,389,316 bytes allocated
```

16 bytes in 1 blocks are definitely lost in loss record 88 of 340 at 0x4C2AB80: malloc (in /usr/lib/valgrind/vgpreload_memcheck-amd64-linux.so) by 0x4O166D: main (in /home/sigvald/mn-fysrp-pic/pinc)

³Since OpenMPI is usually not compiled with -enable-memchecker Valgrind will not be able to detect errors in shared memory space. I guess most (all?) mistakes will be eliminated using the PINC Valgrind wrapper, however.

```
1,048,576 bytes in 1 blocks are definitely lost in loss record 340 of 340
  at 0x4C2AB80: malloc (in /usr/lib/valgrind/vgpreload_memcheck-amd64-linux.so)
  by 0x40164E: test (in /home/sigvald/mn-fysrp-pic/pinc)
  by 0x401685: main (in /home/sigvald/mn-fysrp-pic/pinc)

LEAK SUMMARY:
  definitely lost: 1,048,592 bytes in 2 blocks
  indirectly lost: 0 bytes in 0 blocks
  possibly lost: 0 bytes in 0 blocks
  still reachable: 0 bytes in 0 blocks
  suppressed: 207,280 bytes in 496 blocks
```

For counts of detected and suppressed errors, rerun with: -v ERROR SUMMARY: 2 errors from 2 contexts (suppressed: 53 from 53)

This shows that malloc() in main() allocated 16 bytes which is not freed, and that malloc() in test() in main() allocated 1MiB which is not freed. It also showed that approximately 200KiB which is not freed is suppressed. This is not due to PINC mistake but due to OpenMPI and is therefore not considered an error. Except for the suppressed leaks all leaks should be zero. Feel free to read more about the different leaks online.

The COPT= argument in the make-call above is used to turn off compiler optimizations. Without this, the compiler would figure out that the function test() does nothing and can be omitted. As a result, only the first error would show up. In fact, the second error does not exist any more after optimizing and therefore pose no problems. Nevertheless, it may be helpful to turn off optimizations when looking for memory leaks.

Finally, beware that running Valgrind degrades execution speed.

7.2 GProf

To get an overview of what is time-consuming in PINC, execute the following commands:

```
make clean
make CADD=-pg
./pinc input.ini
```

CADD is used to add additional flags to the compiler. In this case instrumentation code is incorporated into PINC to allow GProf to profile it. Upon execution of PINC the file gmon.out (gitignored) is created which can be analysed with GProf. Extensive documentation of GProf is available online but as an example,

```
gprof -bap pinc gmon.out may return
```

Flat profile:

Each sample counts as 0.01 seconds.

%	cumulative	self		self	total	
time	seconds	seconds	calls	ms/call	ms/call	name
100.04	0.96	0.96	3	320.14	320.14	posUniform
0.00	0.96	0.00	36	0.00	0.00	intArrMul
0.00	0.96	0.00	22	0.00	0.00	iniGetStrArr
0.00	0.96	0.00	14	0.00	0.00	intArrProd
0.00	0.96	0.00	7	0.00	0.00	${\tt iniGetLongIntArr}$
0.00	0.96	0.00	6	0.00	0.00	msg
0.00	0.96	0.00	3	0.00	0.00	${\tt iniGetIntArr}$
0.00	0.96	0.00	2	0.00	0.00	${\tt iniGetDoubleArr}$
0.00	0.96	0.00	1	0.00	0.00	allocGrid
0.00	0.96	0.00	1	0.00	0.00	allocPopulation
0.00	0.96	0.00	1	0.00	0.00	tFormat
0.00	0.96	0.00	1	0.00	0.00	velMaxwell

Mind that a significant amount of time is necessary in order for GProf to be able to determine non-zero time.

7.3 Simple Timing using PINC Timer

Then compiling with

make clean
make

./pinc input.ini

While GProf is suitable to get an idea of the execution of the whole program it has its flaws. One of them is when you want to know rigorously how fast certain operations execute. For this purpose, the PINC Timer datatype may come in handy. Consider for instance that you know two different ways of implementing the same thing, one intuitive way using nested loops, and one "clever" way using one loop and a modulo operator. These can be compared as shown below:

```
Timer *timer = allocTimer(0);
2
3
             int nDims = 3;
             int L[3] = {1,2,4};
4
5
             double *pos = pop->pos;
6
7
             tMsg(timer, NULL);
8
9
             for(long int i=0; i<1e7; i++){
10
                     for (int d=0; d < nDims; d++) {
                              pos[i*nDims+d] = L[d]*
11
                                  gsl_rng_uniform_pos(rng);
12
13
14
15
             tMsg(timer, "Nested loops method");
16
             for(long int i=0; i<nDims*1e7; i++){</pre>
17
18
                     pos[i] = L[i%nDims] * gsl_rng_uniform_pos(rng);
19
20
21
             tMsg(timer, "Modulus method");
22
23
            freeTimer(timer);
```

```
TIMER (0): [tot=332.81ms, diff=289.26ms] Nested loops method TIMER (0): [tot=619.69ms, diff=286.83ms] Modulus method
```

tot shows the time since program start-up whereas diff shows time since previous invocation of tMsg(). tMsg(timer, NULL) can be called simply to reset the timer without printing any message.

In this case, we see that both methods perform equally well at approximately 290 ms. The difference is insignificant. It is interesting though, to re-run the experiments with optimizations turned off ("make CADD=-pg COPT="):

```
TIMER (0): [tot=397.32ms, diff=359.46ms] Nested loops method TIMER (0): [tot=956.03ms, diff=558.67ms] Modulus method
```

It is now evident that the intuitive nested loops method by itself is faster but the compiler has optimized both methods such that they perform similarly. This information, however, is purely for educational purpose, as it is no point in optimizing the code with compiler optimizations turned off. The rationale is; if two alternatives perform equally well with compiler optimizations on, choose the prettiest solution. If not, choose the fastest.

Whereas this example was well optimized by the compiler, this may not always be the case. It is therefore highly advised to think through your programming techniques, and when uncertain as to what will perform well, measure it.

As a final note, although the PINC Timer has a very high resolution the accuracy is more influenced by random variations and overhead when measuring short times. A remedy to this is to put the operations to be measured in a loop to get the timer up to the the millisecond/second range. To get an idea of the resolution, the overhead and the accuracy of tmsg() try measuring tmsg() itself by running it in a loop⁴.

7.4 GNU Debugger (GDB)

GDB may be useful if for instance you want to step through your code, inspecting what's happening to variables as the program run. To be able to use GDB the program must be compiled with the additional -g flag as follows:

```
make clean
make CADD=-g
gdb pinc
```

from which point you can use GDB. GDB is well documented online. Beware that sometimes things may look strange due to optimizations, for instance the value of a variable may not exist and show up as "<optimized out>", either because it simply is not needed, or because it is not needed at this point. As usual, you can turn off optimization for debugging purposes by running make CADD=-g COPT=.

⁴Technically the timer is measured at the beginning of tMsg() and reset at the end of tMsg() such that diff actually shows the time between, but not including, calls to tMsg(). This gives more accurate readings of what comes in between. On my computer tMsg() executes in approximately $5\mu s$ but the overhead of the measurements is only approximately 200 ns. The discrepancy is largely due the fact that printing to the terminal takes time.