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Code_Saturne documentation

***Code_Saturne* version 4.1.1 developer's guide**

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1 Coding style guidelines

1.1 Master rule

Keep the style consistent !

This rule should be observed above all others. The coding style in *Code_Saturne* has evolved over the years, but unless you are ready to update a whole file to a more current style (in which case the other guidelines should be followed), try to remain consistent with the style in the current file.

For new files, use recently updated examples, such as `src/base/cs_field.c` and `src/basecs_field.h` for C, `src/base/field.f90` for Fortran modules, or `src/base/codits.f90` for other Fortran files.

1.2 General rules

The following general rules are strongly recommended:

- Except for files in which they have a special meaning (such as Makefiles), use spaces, not tabs. *Absolutely* avoid this in Python code ¹. Most importantly, use a decent text editor that does not randomly mix spaces and tabs. *Code_Saturne* has a `sbin/rmb` script which removes trailing white-space and replaces tabs with spaces, but this may appear to damage indentation when it was defined with an odd mix of spaces and tabs.
- 80 characters maximum line length; split lines longer than this to ensure readability on small screens, or when viewing code side-by-side on wider screens. This rule is less important for L^AT_EX documentation sources (one could argue that using one line per paragraph and relying on line wrapping would actually make revision merging simpler).

For new developments, prefer C to Fortran, as the code should progressively mve to purely C code. As many variables and arrays are still accessible only through Fortran modules, this is not always possible, but defining Fortran/C bindings such as in the `field.f90` module helps make data accessible to both languages, easing the progressive migration from Fortran to C. Fortran bindings should only be defined when access to C functions or variables from Fortran is required, and may be removed for parts of the code purely handled in C.

1.3 C coding style

1.3.1 Punctuation

Except when adding additional white space to align similar definitions or arguments on several lines, standard English punctuation rules should be followed:

- no white space before a punctuation mark (, ; .), one white space after a punctuation mark.
- white space before an opening parenthesis, no white space after an opening parenthesis.
- no white space before a closing parenthesis, white-space after a closing parenthesis.

1.3.2 General rules

The following presentation rules are strongly recommended:

- indentation step: 2 characters (4 characters in `cs_gui.*` files).

¹Keeping to Python's humoristic example style, anybody doing this should learn "how not to be seen"

- always use lowercase characters for instructions and identifiers, except for enumerations and macros which should be in uppercase.

The following coding rules are strongly recommended:

- header (`.h`) files should have a mechanism to prevent multiple inclusions;
- all macro parameters must be enclosed inside parentheses;
- a function's return type must always be defined.
- variables should be initialized before use (pointers are set to `NULL`). A good compiler should issue warnings when this is not the case, and those warnings must be acted upon;
- when a structure definition is only needed in a single file, it is preferred to define it directly in the C source file, so as to make as little visible as possible in the matching header file. structures only used through pointers may be made opaque in this manner, which ensures that their possible future modification should not have unexpected side-effects.
- When a public function is defined in a C source file, a matching header file containing its prototype must be included.
- usage of global variables must be kept to a minimum, though such variables may be useful to maintain state or references to mesh or variable structures in C code callable by Fortran code. If a global variable is only needed inside a single file, it should be declared "static". If it is needed in other files, then it must instead be declared "extern" in the matching header file.
- a `const` type must not be cast into a non-`const` type;
- every `switch` construct should have a `default` clause (which may reduce to `assert(0)` to check code paths in debug mode, but at least this much must be ensured);
- a `const` attribute should be used when an array or structure is not modified. Recall that for example `const cs_mesh_t *m` means that the contents of mesh structure `m` are not modified by the function, while `cs_mesh_t *const m` only means that the pointer to `m` is not modified; `const cs_mesh_t *const m` means both, but its usage in a function prototype gives no additional useful information on the function's side effects than the first form (`const cs_mesh_t *m`), so that form is preferred, as it does not clutter the code;
- when an array is passed to a function, describing it as `array[]` is preferred to `*array`, as the array nature of the argument is better conveyed.
- where both a macro or an enumerated constant could be used, an enumeration is preferred, as values will appear with the enumerated value's name under a debugger, while only a macro's expanded value will appear. An additional advantage of enumerated values is that a compiler may issue a warning when a `switch` construct has no `case` for a given enumeration value.

1.3.3 Language

ANSI C 1999 or above is required, so C99-specific constructs are allowed, though C++ style comments should be avoided, so as to maintain a consistent style. C99 variable-length arrays should be avoided, as it is not always clear whether they are allocated on the stack or heap, and are an optional feature only in the C newer 2011 standard (though we could expect that support for those constructs will remain available on general-purpose architectures, and removed only in the embedded space).

1.3.4 Assertions

Assertions are conditions which must always be verified. Several expanded macro libraries may be available, but a standard C language assertion has the following properties:

- it is only compiled in debug mode (and so incur no run-time performance penalty in production code, where the `NDEBUG` macro is defined);
- when its predicate are not verified, it causes a core dump; when running under a debugger, the code is stopped inside the assertion, but does not exit, which simplifies debugging.

Assertions are thus very useful to ensure that conditions which are always expected (and not dependent on program input) are met. They also make code more readable, in the sense that it is made clear that conditions checked by an assertion are always expected, and that not handling other cases is not an programming error or omission.

If a condition may not be met for some program inputs, and not just in case of programmer error, a more complete test and call to an error handler (such as `bft_error`) is preferred.

1.4 Naming conventions

The following rules should be followed:

- identifier lengths should not exceed 31 characters if avoidable; this was a portability requirement using C89, and is now more a readability recommendation;
- identifier names are in lowercase, except for macro or enumeration definitions, which are in uppercase; words in an identifier are separated by an underscore character (for example, `n_elt_groups`).
- global identifier names are prefixed by the matching library prefix, such as `cs_` or `BFT_`;
- local identifiers should be prefixed by an underscore character.
- Index arrays used with 0 to $n - 1$ numbering should be named using a `idx_` or `index_` prefix or suffix, while similar arrays using a 0 to $n - 1$ numbering (usually those that may be also used in Fortran code) should be named using a `pos_` prefix or suffix.

1.4.1 Naming of enumerations

The following form is preferred for enumerations:

```
typedef myclass { CS_MYCLASS_ENUM1,
                  CS_MYCLASS_ENUM2,
                  /* etc. */
                  } cs_myclass_t;
```

1.4.2 Naming of structures and associated functions

Macros and enumerations related to myclass structures are prefixed by `CS_MYCLASS_`.

Public functions implementing methods are named `cs_class_method`, while private functions are simply named: `_class_method` and are declared static.

Files containing these functions are named `_class.c`.

1.4.3 Integer types

Several integer types are found in *Code_Saturne*:

- `cs_lnum_t` should be used for local entity (i.e. vertex, face, cell) numbers or connectivity. It is a signed integer, normally identical to `int`, but a larger size could be used in the future for very large meshes on shared memory machines.
- `cs_gnum_t` should be used for global entity numbers, usually necessary only for I/O aspects. It is an unsigned 32 or 64-bit integer, depending on whether the code was configured with the `--enable-long-gnum` option. Global numbers should always use this type, as for very large meshes, they may exceed the maximum size of a 32-bit integer (2 147 483 648). The choice of unsigned integers is two-fold: it doubles the range of available values, and good compilers will issue warnings when this type is mixed without precaution with the usual integer types. These warnings should be heeded, as they may avoid many hours of debugging.
- `cs_int_t` is deprecated; it was used for integer variables or arrays passed between C and Fortran, though using `integer(kind)` statements in Fortran should be a better future solution. In practice, `cs_int_t` and `cs_lnum_t` are identical. The former is more commonly found in older code, but the latter should be used where applicable for better clarity.
- in all other cases, the standard C types `int` and `size_t` should be preferred (for example for loops over variables, probes, or any entity independent of mesh size).

1.5 Base functions and types

In the *Code_Saturne* kernel, it is preferable to use base functions provided by the BFT subsystem to the usual C functions, as those logging, exit and error-handling functions will work correctly when running in parallel, and the memory management macros ensure return value checking and allow additional logging.

The array below summarizes the replacements for usual functions:

C function	<i>Code_Saturne</i> macro or function	Header
<code>exit()</code>	<code>cs_exit()</code>	<code>cs_base.h</code>
	<code>bft_error()</code>	<code>bft_error.h</code>
<code>printf()</code>	<code>bft_printf()</code>	<code>bft_printf.h</code>
<code>malloc()</code>	<code>BFT_MALLOC()</code>	<code>bft_mem.h</code>
<code>realloc()</code>	<code>BFT_REALLOC()</code>	<code>bft_mem.h</code>
<code>free()</code>	<code>BFT_FREE()</code>	<code>bft_mem.h</code>

1.6 Internationalization

Internationalization of messages uses the `gettext()` mechanism. Messages should always be defined in US English in the source code (which avoids using extended characters and the accompanying text encoding issues in source code), and a French translation is defined and maintained using a translation file `po/fr.po`. Translations to other languages are of course possible, and only require a volunteer.

Using the `gettext()` mechanism has several advantages:

- accented or otherwise extended characters appear normally whether using a Latin-1 (or Latin-9 or Latin-15) environment or whether using a “Unicode” (or generally UTF-8) environment (assuming that a terminal's encoding matches that of the `LANG` environment variable, usually `LANG=fr_FR` or `LANG=fr_FR.UTF-8` for French;
- if a message is not translated, it simply appears in its untranslated version;

- maintenance of the translations only requires editing a single file, gettext related tools also make it easy to check that translations are consistent (i.e. matching format descriptors or line returns) without requiring complete code coverage tests. In fact, translations could be maintained by a non-programmer.
- internationalization may be disabled using the `--disable-nls` configure option, so possible comfort vs. speed trade-offs may be decided by the user;

To make internationalization possible, translatable strings should be encased in a `_()` macro (actually an abbreviation for a call to `gettext()` if available, which reverts to an empty (identity) macro if internationalization is unavailable or disabled). Strings assigned to variables must be encased in a `N_()` macro (which is an “empty” macro, used by the `gettext` toolchain to determine that those strings should appear in the translation dictionary), and the variable to which such a string is assigned should be encased in the `_()` macro where used.

Note that with UTF-8 type character strings, accented or otherwise extended characters are represented on multiple bytes. The `strlen()` C function will return the string's real size, which may be greater than the number of output columns it uses. In the preprocessor, the `ecs_print_padded_str()` may be used to print such a string and padding it with the correct number of white spaces so as to meet a given format width. No such function is used or currently needed in the main code, though it could be added if needed.

1.7 Fortran coding style

1.7.1 Conventions inherited from Fortran 77

The following coding conventions were applied when the code used Fortran 77, prior to conversion to Fortran 95. Some of them should be updated, as long as we maintain consistency within a given file.

- one routine per file (except if all routines except the first are “private”). This rule has a few exceptions, such as in modules, in the `cs_user_parameters.f90` user file which contains several subroutines (it initially followed the rule, but subroutines were split, while the file was not), and Fortran wrappers for several C functions defined in a single C file are also usually defined in a single source, as they are a consistent whole.
- exactly 6 characters per routine name, with no underscores. As Fortran 95 allows longer identifiers, the 6 character limit is obsolete, but avoiding `_` characters is still recommended in routines that might be called from C, unless `bind(C)` is used, as most compilers add an underscore character to the routine name, and often add a second underscore if no special options are given, while the `C CS_PROCF` macro does not handle this situation, possibly leading to link issues. For routine names longer than 6 character, more verbose names are recommended (using underscores as word separators), though the Fortran 95 standard requires those names be limited to 31 characters. Also, for routine names with underscores, the `CS_PROCF` macro must not be used. ISO C bindings must be used instead.
- at least 2 characters per variable names (banish variables `i`, `j`, or `k`, preferring `ii`, `jj`, or `kk`, as this makes searching under a text editor easier for non-experts).
- avoid commented example lines in user subroutines; otherwise, the code is never compiled and thus probably incorrect. Using a `if (iuse) ... endif` construct with `iuse = 0` instead is recommended.
- use `do / enddo` constructs instead of `do / continue`.
- avoid `goto` constructs where `select / case` would be more appropriate.
- avoid print statements using `write(format, *)`, or `print` constructs, to ensure that output is redirected correctly in parallel mode.

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- use `d` and not `e` to define double-precision floating-point constant definitions. Especially avoid constants with exponents such as `e50`, which are impossible in single precision (the limit is `e38`), and may thus not be accepted by “strict” compilers, or worst, lead to run-time exceptions.

1.7.2 Language

Fortran 1995 or above is required, and constructs or intrinsic functions requiring Fortran 2003 or above should be avoided, except for the Fortran 2003 ISO_C_BINDING module, which is available in all major current Fortran compilers.

1.8 Python coding style

The GUI is not yet compatible with Python 3, due to differences in the usual PyQt4 API and strings/unicode handling, but the rest of the Python code should work both with Python 2 and Python 3. This compatibility should be maintained or improved upon, not broken...

Details on the differences between major Python versions and associated recommendations may be found at: <http://docs.python.org/py3k/howto/pyporting.html>.

2 Common construct types

In this chapter, commonly-used construct types whose use may require specific explanations or recommendations are described.

2.1 Indexed arrays

In many instance data such as mesh connectivity requires managing a variable number of entries per data element. This is for example the case of *faces* \rightarrow *vertices* connectivity. The average number of vertices per face is usually quite low, but the maximum number may be significantly higher, so using an array with regular stride would be very inefficient for some data sets.

A common solution to this problem is to use indexed arrays, in which an array containing data is supplemented by a second array containing the start indexes of entries in the data array for each element.

These arrays are mainly used in the C parts of the *Code_Saturne* source, though the interior and boundary *faces* \rightarrow *vertices* connectivity is also visible in the Fortran code. Remember that in Fortran code, arrays are always one-based (i.e. the first element of an array has index 1), while in C code, the natural indexing is zero-based, but one-based indexing may also be used for arrays visible from Fortran code, or for arrays using global numbers. In *Code_Saturne*, zero-based indexes are often used with one-based data, for example when defining element connectivities, where element ids are usually one-based². For C code, when there are no mapping constraints due to Fortran, the recommendations are the following:

- local index arrays should be zero-based.
- global index arrays should be one-based. This should only concern indexes read from or written to file.
- when containing cell, face, or vertex connectivity information, data arrays may be either zero or one-based: zero based arrays are less error-prone so they should be preferred, but where element ids may be signed (so as to convey orientation information), one-based arrays are necessary. In a given structure, consistency is recommended, so if a *cells* \rightarrow *faces* connectivity requires one-based face numbers, an associated *faces* \rightarrow *vertices* connectivity may also use one-based vertex numbers, even though vertices have no orientation.

Let us consider an array `array_data` indexed by a zero-based `array_index` array. The values of `array_data` associated with element i_e , are the values ranging from indexes $i_{start} = i_e$ included to $i_{end} = i_e + 1$ excluded (past-the-end index).

The number of values associated with i_e is determined by: $\text{par } \text{array_index}[i_e + 1] - \text{array_index}[i_e]$, whether the index is zero-based or one-based.

For an indexed array of n elements, the size the index array should thus be equal to $n + 1$ (and not n as would be the case for regular 1-d or strided arrays), and the total size of `array_data` is equal to `array_index[n]` for a zero-based index, or `array_index[n] - array_index[0]` in general.

2.1.1 similar popular data structures

Readers familiar with *Compressed Sparse Row* or similar matrix or graph representations may already have noted the similarity with the indexed arrays described here. In the case of CSR matrix structures, 2 data arrays are often associated with 1 row index: one array defining the column indices, and a second one defining the associated values.

²both as a convention to simplify mapping to Fortran, and in the case of *cells* \rightarrow *faces* connectivities, so as to use the sign to determine face orientation

This is in reality no different than using an indexed array as described here to define a *faces* \rightarrow *vertices* connectivity, and also associating data (for example coordinates) to vertices.

In *Code_Saturne*, matrix non-diagonal terms usually correspond to cell faces, and the CSR matrix representation is very similar to that of a *cells* \rightarrow *faces* connectivity, except for the fact that a standard CSR representation uses only “unsigned” column ids, whereas face numbers may be signed in the matching mesh representation so as to convey orientation (an alternative solution would be to use a separate array for orientation, in which case the similarity to CSR would be complete).

2.1.2 Indexed Array Example

We illustrate the use of an indexed array to define a *faces* \rightarrow *vertices* connectivity for a simple surface mesh:



The matching arrays are:



Let us now assume that we need to keep track of the association between faces and some specific areas of the mesh. Continuing on the same example, consider a single group of interest, with id 1, with which the left part of the mesh (i.e. on the quadrangles), is associated. The *faces* \rightarrow *zones* connectivity is the defined as follows:



This example, in which the right-side elements (i.e. the triangles) belong to no specified group illustrates how elements with no associated data are handled: their index and that of the following element is simply the same.

3 Write a part of the theory guide

3.1 General rules

Theses general rules should be seen as basic golden rules helping the whole documentation to be consistent. They are strongly recommended:

- Respect a plan where you first present a general overview of the theory (what is it about, what is the main goal), then you present the equations in general, and finally the specific choices you have made.
- Use the macros described in § 3.2 (*i.e.* `\usepackage{csmacros}`).
- Use the notations defined in the nomenclature of the theory guide as much as possible.
- Focus on your specificities and cite the generalities (external to EDF!), which you should add to the `biblio.bib` file located in the `/doc/style/` directory.
- Write in English (UK).
- Use the existing style of *Code_Saturne*, that is to say use the class `csdoc.cls` (for long documents as a report) or the class `csshortdoc.cls` (for short documents as an article).
- Respect L^AT_EX philosophy, as it is designed to make sensible spacing decisions by itself, do not use explicit horizontal or vertical spacing commands, except in a few accepted (mostly mathematical) situation.
- keep your own macros to an absolute minimum.

3.2 Macros and typos

This section does not pretend to discibe how to write a L^AT_EX document, but is to present the macros defined in `csmacro.sty` and give some typographic pieces of advice.

3.2.1 Macros

The available macros located in the `csmacros` and `csvers.tex` package are displayed in Table 1 and Table 2.

3.2.2 Typography

Here are some usefull tricks:

- If you want to make a description many topics, use the `\begin{itemize} \item \end{itemize}` environment.
- You can use blue and orange EDF colours with the blue `\textcolor{blueedf}{text}`, its the darkened version `\textcolor{bluededf}{text}`, or the orange `\textcolor{orangeedf}{text}` and its the darkened version `\textcolor{orangededf}{text}`.
- Use label and references, and dissociate equations with sections and appendices and figures and tables using `\label{eq:label}`, `\label{sec:label}`, `\label{ap:label}`, `\label{fig:label}` and `\label{tab:label}` prefixes.
- Use the `\emph{}` mode for acronyms (*e.g.* EDF).
- Use the `\emph{}` mode for Latin words(*e.g.*, *i.e.*, *a priori*, *etc.*).

L ^A T _E Xcode	preview
<code>\CS</code>	<i>Code_Saturne</i>
<code>\ensight</code>	EnSight
<code>\ensightg</code>	EnSight Gold
<code>\fluent</code>	FLUENT
<code>\bft</code>	BFT
<code>\fvm</code>	FVM
<code>\gambit</code>	GAMBIT
<code>\gmsh</code>	Gmsh
<code>\harpoon</code>	Harpoon
<code>\hexpress</code>	<i>HexPress</i>
<code>\icemcfd</code>	ICEM CFD
<code>\ideas</code>	I-deas
<code>\med</code>	MED
<code>\metis</code>	METIS
<code>\parmetis</code>	PARMETIS
<code>\nopo</code>	NOPO
<code>\paraview</code>	ParaView
<code>\pcs</code>	Preprocessor
<code>\salome</code>	SALOME
<code>\scotch</code>	SCOTCH
<code>\ptscotch</code>	PT-SCOTCH
<code>\simail</code>	SIMAIL
<code>\starcd</code>	STAR-CD
<code>\starccmp</code>	STAR-CCM+
<code>\syrrhes</code>	SYRTHES
<code>\vtk</code>	VTK

Table 1: Macros of softwares defined in `csmacros.sty`.

L ^A T _E Xcode	preview
<code>\$\$\divs\$</code>	div
<code>\$\$\divv\$</code>	div
<code>\$\$\divt\$</code>	$\underline{\text{div}}$
<code>\$\$\grad\$</code>	∇
<code>\$\$\gradv\$</code>	∇
<code>\$\$\gradt\$</code>	$\underline{\nabla}$
<code>\$\$\rot\$</code>	rot
<code>\$\$\vect{V}\$</code>	\underline{V}
<code>\$\$\tens{T}\$</code>	$\underline{\underline{T}}$
<code>\degresC</code>	$^{\circ}\text{C}$
<code>\$\$\Max\$</code>	Max
<code>\$\$\Min\$</code>	Min
<code>\$\$\trace\$</code>	<i>tr</i>
<code>\$\$\transpose{M}\$</code>	M^T
<code>\$\$\deviator{M}\$</code>	M^D
<code>\$\$\symmetric{M}\$</code>	M^S
<code>\$\$\dd\$</code>	d

Table 2: Macros of some mathematical symbols defined in `csmacros.sty`.

L ^A T _E Xcode	preview
<code>Facei{celli}</code>	\mathcal{F}_i^{int}
<code>Faceb{cellj}</code>	\mathcal{F}_j^{ext}
<code>Face{celli}</code>	\mathcal{F}_i
<code>fij</code>	f_{ij}
<code>fib</code>	f_b
<code>ij</code>	ij
<code>ib</code>	ib
<code>celli</code>	i
<code>cellj</code>	j
<code>ipf</code>	I'
<code>jpf</code>	J'
<code>centi</code>	I
<code>centj</code>	J
<code>centip</code>	I'
<code>centjp</code>	J'
<code>cento</code>	O
<code>centf</code>	F

Table 3: Macros of discretized quantities defined in `csmacros.sty`.

- Use `\left(` instead of `(` and `\right)` instead of `)` in math mode.
- DO NOT put a space before the symbol “:”. In English the rule is no space, never.
- DO NOT use `\newline` or `\\` except in a tabular environment or an array.
- Write “Equation” with a first upper case letter. Use `\figurename~` and `\tablename~` write Figure and Table.
- Use the enumerate environment:

```

\begin{enumerate}[label=\roman{*}/, ref=(\roman{*})]
\item $1^{st}$ item
\item $2^{nd}$ item
\end{enumerate}

```

i/ 1st item

ii/ 2nd item

- Use the remarks `\begin{remark}` `\end{remark}` and example `\begin{example}` `\end{example}` environments defined in `csdoc.csl`:

Remark 3.1 *A remark*

Example 3.1 *An example*