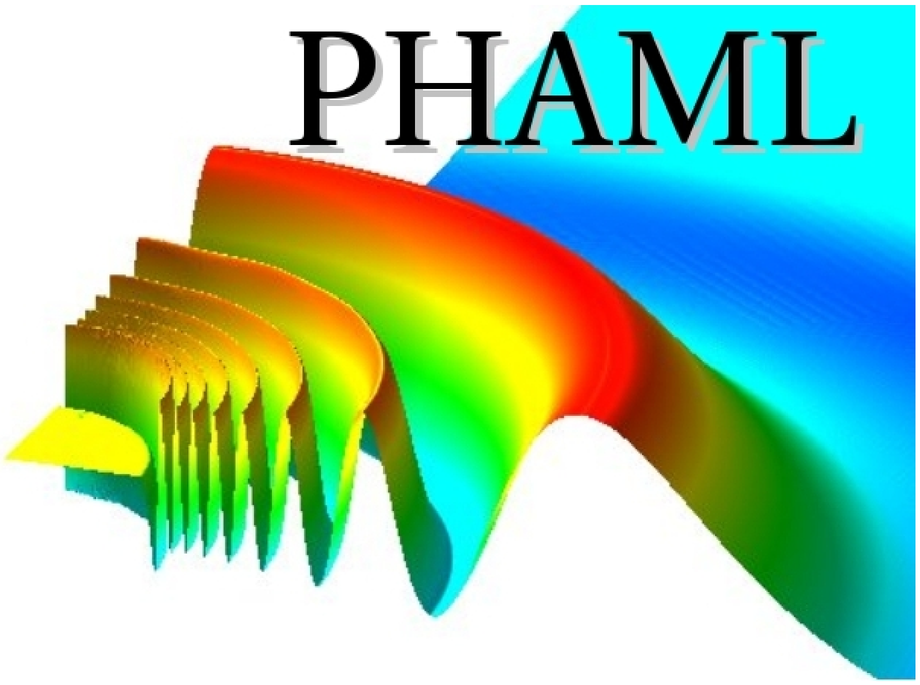
NISTIR 7374

PHAML User's Guide

William F. Mitchell
U. S. Department of Commerce
Technology Administration
National Institute of Standards and Technology
Information Technology Laboratory
Gaithersburg, MD 20899 USA

Revised August 28, 2018 for Version 1.20.0



PHAML User's Guide, Version 1.20.0

William F. Mitchell[1]
Applied and Computational Mathematics Division
100 Bureau Drive Stop 8910
National Institute of Standards and Technology
Gaithersburg, MD 20899-8910
email: phaml@nist.gov

[1]Contribution of NIST, not subject to copyright in the United States. The mention of specific products, trademarks, or brand names is for purposes of identification only. Such mention is not to be interpreted in any way as an endorsement or certification of such products or brands by the National Institute of Standards and Technology. All trademarks mentioned herein belong to their respective owners.

Abstract

PHAML (Parallel Hierarchical Adaptive MultiLevel) is a Fortran module for the solution of elliptic partial differential equations. It uses finite elements, adaptive grid refinement (h, p or hp) and multigrid solution techniques in a message passing parallel program. It has interactive graphics via OpenGL. This document is the user's guide for PHAML. The first part tells how to obtain any needed software, how to build and test the PHAML library, and how to compile and run the example programs. The second part explains the use of PHAML, including program structure and the various options that are available. The third part is a reference manual which describes the API (application programming interface) of PHAML. The reference manual begins with a 2 page Quick Start section for the impatient.

Keywords: adaptive grid refinement, dynamic load balancing, elliptic eigenvalue problems, elliptic partial differential equations, high order finite elements, hp-adaptivity, multigrid, parallel programming

Contents

Chapter 1

Introduction

To start using PHAML immediately, see the Quick Start guide in Section 6.1.

PHAML stands for Parallel Hierarchical Adaptive MultiLevel method. It solves systems of linear elliptic partial differential equations (PDEs) of the form

$$-\frac{\partial}{\partial x}\left(c_{xx}\frac{\partial u}{\partial x}\right)-\frac{\partial}{\partial x}\left(c_{xy}\frac{\partial u}{\partial y}\right)-\frac{\partial}{\partial y}\left(c_{yy}\frac{\partial u}{\partial y}\right)+c_x\frac{\partial u}{\partial x}+c_y\frac{\partial u}{\partial y}+c_u u=f \quad \text{in } \Omega \tag{1.1}$$

where c_{xx}, c_{xy}, c_{yy}, c_x, c_y, c_u and f are functions of x and y, and the domain Ω is a bounded, connected, region in R^2. The boundary conditions can be Dirichlet on part of the boundary,

$$u \;=\; g \quad \text{on } \partial\Omega_D \tag{1.2}$$

and natural or mixed on the remainder of the boundary,

$$\left(c_{xx}\frac{\partial u}{\partial x}+c_{xy}\frac{\partial u}{\partial y}\right)\frac{\partial y}{\partial s}-c_{yy}\frac{\partial u}{\partial y}\frac{\partial x}{\partial s}+c_{bc}u \;=\; g \quad \text{on } \partial\Omega_N \tag{1.3}$$

where g and c_{bc} are functions of x and y, c_{xx}, c_{xy} and c_{yy} are the same functions as in Equation 1.1, and the boundary $\partial\Omega = \partial\Omega_D \cup \partial\Omega_N$ and $\partial\Omega_D \cap \partial\Omega_N = \emptyset$. Periodic boundary conditions are also supported.

For natural boundary conditions, differentiation with respect to s is with respect to a counterclockwise parameterization of the boundary $(x(s), y(s))$ with $\|(dx/ds\ dy/ds)\| = 1$. Note that when $c_{xx} = c_{yy} = 1$ and $c_{xy} = 0$ or the boundaries of the domain are parallel to the axes, the natural boundary condition reduces to the Neumann boundary condition

$$\frac{\partial u}{\partial n} \;=\; g$$

where n is the outward unit normal.

If the domain has curved boundaries, it is defined by subroutines that define the boundary parametrically. If it is polygonal, it can instead be defined by an initial triangulation given in data files created by the program Triangle.

PHAML also solves elliptic eigenvalue problems where the right hand side $f(x, y)$ is λu, and λ is an eigenvalue to be determined along with u. For eigenvalue problems, the boundary conditions must be homogeneous, i.e., $g = 0$.

PHAML also solves 3D elliptic PDEs, with the obvious extensions to Equations 1.1 and 1.3. See Section 4.4. Most of the rest of the user's guide will only address the 2D problem.

PHAML discretizes the PDE using the standard finite element method with piecewise polynomial functions over triangles. The approximating polynomial degrees may be a fixed constant or adaptive. The grid is generated by beginning with a very coarse grid of fixed degree and using uniform or adaptive h-refinement in the form of newest node bisection, uniform or adaptive p-refinement in which the polynomial degree is increased, or hp-adaptive refinement which combines both forms of refinement.

The standard process alternates between phases of grid adaptation and solution of the discrete equations. The default solution method is a hierarchical basis multigrid method. Other solution methods are available through other optional software packages. If the cross derivative or first order terms are included, i.e. $c_{xy} \neq 0$, $c_x \neq 0$ or $c_y \neq 0$, then one of the alternate solution methods for nonsymmetric matrices must be used. All this is performed in parallel using the full domain partition to minimize communication. The default load balancing method is a refinement-tree based partitioning algorithm. Other load balancing methods are available through other optional software packages.

PHAML can be run as a sequential program, a master/slave parallel program using MPI-2, an SPMD parallel program using MPI-1, MPI-2, an SMP program using OpenMP, or a hybrid parallel program using both MPI and OpenMP. PHAML optionally uses OpenGL to provide menu-driven interactive visualization.

Chapter 2

Software

2.1 Obtaining Software

PHAML and all required or optional auxiliary software can be obtained by freely downloading them from the web, although some have commercial alternatives. This section explains what software is used with PHAML, when you need that software, and where to obtain it. Most of this software is optional and you do not need to install it unless you are using the relevant features as described below.

2.1.1 PHAML

PHAML is available for download at `http://math.nist.gov/phaml`. It is a gzipped tar file. When unpacked, it creates a directory called `phaml-x.x.x` where the x's are the version number. It has been tested under many Unix systems, but not under MS Windows. It is standard conforming Fortran 90, so (theoretically) it should work under Windows (at least sequentially) without too much effort. For the remainder of this document, we will assume that the operating system is some variant of Unix, including Linux.

2.1.2 Fortran 90 and C Compilers

A Fortran 90 (or later Fortran standard) compiler is required to compile PHAML. In some cases, a C compiler will also be required to compile some wrapper routines to C libraries. Most Unix systems already have a C compiler installed, and many also have a Fortran 90 compiler installed. Check your local documentation to find out, or look for a command like f90 or f95.

If you do not have a Fortran 90 compiler, many good commercial compilers are available for most (if not all) Unix systems. To identify what is available for your system, see Michael Metcalf's *Fortran 90/95/HPF Information File* at `http://www.fortran.com/fortran/metcalf.htm`.

There are currently two free Fortran 90 compilers, g95 at `http://www.g95.org` and GNU's gfortran at `http://gcc.gnu.org/fortran`.

2.1.3 BLAS and LAPACK

BLAS (Basic Linear Algebra Subroutines) and LAPACK (Linear Algebra PACKage) libraries are required for PHAML. The reference Fortran implementation for them can be obtained from Netlib at `http://www.netlib.org`. However, for best performance you should use a BLAS library that is optimized for your computer system. You may find that the BLAS and LAPACK libraries are already installed on your system, or that there are commercial optimized versions available for your system.

There are also freely available optimized BLAS packages such as ATLAS at `http://math-atlas.sourceforge.net` and GOTO BLAS at `http://www.tacc.utexas.edu/resources/software/`.

2.1.4 MPI

To run PHAML as a message passing parallel program, you must have an MPI library. Many computer systems will already have an MPI library installed. Check your local documentation. If not, there are freely available implementations of MPI. The Open MPI implementation is available at `http://www.open-mpi.org`. The MPICH implementation is available at `http://www.mpich.org`.

2.1.5 OpenGL (or Mesa), GLUT and f90gl

If you wish to use the visualization capabilities of PHAML, then you will need an OpenGL library (graphics library), GLUT (window, mouse, keyboard and menu management), and f90gl (the Fortran 90 interface to OpenGL and GLUT).

Some computers will already have an OpenGL library installed. If not, there are some commercial OpenGL libraries for some computer systems, and there is the freely available Mesa library. Mesa can be obtained from `http://www.mesa3d.org`, and further information about OpenGL can be found at `http://www.opengl.org`.

If your system already has an OpenGL library, then it is likely to also have GLUT already installed. However, many versions of GLUT are not compatible with f90gl, so you may need to reinstall GLUT anyway. If you (re)install GLUT, you should get it from the software section of the f90gl web pages at `http://math.nist.gov/f90gl`. Alternatively, if you are installing Mesa, then also get MesaGLUT. This distribution works with f90gl since version 7.0.3.

It is highly unlikely that f90gl will already be installed on your system. You can obtain f90gl from `http://math.nist.gov/f90gl`.

2.1.6 Triangle

PHAML uses Jonathan Richard Shewchuk's mesh generator, Triangle [42], to generate the initial grid for arbitrary geometry in 2D. If you are only solving problems on the unit square, then you do not need Triangle – you can use the Triangle output files in the examples. You also do not need it if you have obtained Triangle data files elsewhere. Otherwise, you will need it. You also need it if you choose to define your domain through subroutines. Triangle is available at `http://www.cs.cmu.edu/~quake/triangle.html`.

2.1.7 Gmsh

PHAML uses Gmsh [19, 20] to generate the initial grid for arbitrary geometry in 3D. If you are only solving problems on the unit cube, then you do not need Gmsh – you can use the Gmsh `.msh` files in the examples. You also do not need it if your domain has only planar faces and you have obtained `.msh` files elsewhere. Otherwise, you will need it. Gmsh is available at `http://geuz.org/gmsh`.

2.1.8 SLEPc

To solve elliptic eigenvalue problems, PHAML needs an algebraic eigensolver. SLEPc [11] is used for this. SLEPc requires that you also have PETSc (sect. 2.1.11) installed. You can get SLEPc from `http://www.grycap.upv.es/slepc`, but see the note about compatibility in the PETSc section.

2.1.9 ARPACK

ARPACK [25] is an external package supported by SLEPc, and can be used as an eigensolver for PHAML, accessed through SLEPc. It is optional, but if you choose to include it, ARPACK is compiled separate from SLEPc, and you must enable ARPACK support when you configure SLEPc for compilation. You can get ARPACK and PARPACK from `http://www.caam.rice.edu/software/ARPACK`. For a sequential compilation you do not need PARPACK.

2.1.10 BLOPEX

BLOPEX [23, 24] is an external package supported by SLEPc, and can be used as an eigensolver for PHAML, accessed through SLEPc. It is optional, but if you choose to include it, BLOPEX is compiled with SLEPc by using `--download-blopex` when you configure SLEPc for compilation.

2.1.11 PETSc

PETSc [7][8] is a package of iterative linear system solvers and preconditioners from Argonne National Laboratory. In most cases it is not required, but can be linked with PHAML to provide alternative linear system solvers. It is required for 3D problems and for problems that have first order derivative terms or mixed derivative terms. It is available at `http://www.mcs.anl.gov/petsc/`.

However, in the past PETSc has often made changes to the API that require changes in PHAML. Since PHAML is no longer under development, it is possible that a version of PETSc released after the final release of PHAML will not work with PHAML. If you find this to be the case, you can obtain the last version of PETSc known to work with PHAML from the PHAML web page `http://math.nist.gov/phaml`. Note that if you get PETSc from there, you must also get SLEPc from there (if you use SLEPc) because the SLEPc version must agree with the PETSc version.

2.1.12 MUMPS

MUMPS [3][4] is a parallel direct linear system solver. It is not required, but can be included to provide an alternative linear system solver. It is accessed through PETSc, so you must also install PETSc and use `--download-mumps --with-mumps-serial --with-mpiuni-fortran-binding=0` when configuring PETSc for a sequential compilation, or `--download-mumps --download-parmetis --download-scalapack --download-blacs` when configuring PETSc for a parallel compilation.

2.1.13 SuperLU

SuperLU [26] is a parallel direct linear system solver from the Lawrence Berkeley National Laboratory. It is not required, but can be included to provide an alternative linear system solver. It is accessed through PETSc, so you must also install PETSc and use `--download-superlu` for a sequential compilation or `--download-superlu_dist --download-parmetis` for a parallel compilation when configuring PETSc.

2.1.14 *hypre*

hypre [16][17] is a package of iterative linear system solvers and preconditioners from the Lawrence Livermore National Laboratory. It is not required, but can be included to provide alternative linear system solvers. It is accessed through PETSc, so you must also install PETSc and use `--download-hypre` when configuring PETSc.

2.1.15 ML

ML provides multi-level, multigrid-like preconditioners. It is part of the Trilinos Project [50] at Sandia National Laboratory. It is not required, but can be included to provide an alternative AMG preconditioner. It is accessed through PETSc, so you must also install PETSc and use `--download-ml` when configuring PETSc.

2.1.16 Zoltan

Zoltan [14][15] is a library of dynamic load balancing methods. It is not required, but can be linked with PHAML to provide alternative methods for partitioning the grid for distribution over parallel processors. It can be obtained at `http://www.cs.sandia.gov/Zoltan`.

Zoltan may be compiled with suppport for certain third party libraries. Two of these are supported in PHAML through Zoltan. ParMETIS is a static partitioning library. Zoltan includes a complimentary copy of the ParMETIS software. DRUM is utility for load balancing on heterogeneous or dynamically changing parallel computers. It has not yet been officially released and can only be obtained by requesting it from the author.

2.2 Compiling PHAML

This section gives instructions for compiling the PHAML library. Throughout this section it is assumed that the current working directory is the PHAML root directory.

2.2.1 Creating the Makefiles

Before compiling you must create a `Makefile`. The is done by running the shell script `mkmkfile.sh`. This script will make all the `Makefile`s in all the PHAML subdirectories, so you do not need to run any of the other `mkmkfile.sh`s. Before running this script you must edit it to set system dependent values, like the paths to certain libraries, and specify the configuration you wish to build a `Makefile` for (what kind of computer, what message passing library, etc.). Instructions for modifying `mkmkfile.sh` are contained in the file, but are also summarized here. There are three steps to modifying `mkmkfile.sh`: 1) set the default system configuration, 2) set the paths, library names, etc., and 3) set values for particular systems.

In step 1, the default system configuration is set. If you will only be running in one environment, then you can set the configuration here and forget it. In fact, you can probably just make the `Makefile` once and forget it. If you will be using more than one environment, then you can set the defaults here, and they can be overridden by one of the methods described later in this section.

The configuration variables (e.g. `PHAML_ARCH`) and legitimate values (e.g. `origin`) can be found under Step 1 in `mkmkfile.sh`. You can also get a list of all the configuration variables, their legitimate values, and current defaults by executing

```
./mkmkfile.sh help
```

They are:

- `PHAML_ARCH mac origin rs6k sgi sun tflop x86`. This defines the type of computer architecture you have.

- `PHAML_OS aix cougar cygwin irixn32 irix64 linux osx solaris`. This defines the operating system running on your computer.
- `PHAML_F90 absoft g95 gfortran intel lahey mingw nag pathscale pgi sgi sun xlf`. This defines the Fortran 90 compiler to use.
- `PHAML_C cc gcc`. This defines the C compiler to use.
- `PHAML_HASHSIZE 1 2`. This defines the size of hash key to use for global identifiers. `1` uses one integer and `2` uses two integers. Using `1` saves memory and reduces message sizes; using `2` allows smaller elements (more refinement levels).
- `PHAML_PARALLEL messpass_spawn messpass_nospawn openmp hybrid_spawn hybrid_nospawn sequential`. This defines the type of parallelism. You can select between running a sequential program (no parallelism), having a master process that spawns the slave and graphics processes, running an SPMD (single program multiple data) program in which all processes are identical and started from the command line, running an SMP program using OpenMP, and running a hybrid OpenMP/MPI program either as master/slave or SPMD. Note: not all compilers support OpenMP.
- `PHAML_PARLIB lam mpi mpich mpich2 myrinet openmpi none`. This defines the parallel library to use. `lam`, `mpich`, `mpich2` and `openmpi` refer to the packages by those names, `mpi` to vendor implementations of MPI, `myrinet` to a special implementation of MPICH for myrinet networks, and `none` should be used if `PHAML_PARALLEL` is `sequential` or `openmp`.
- `PHAML_ELEMENT triangle tetrahedron tetrahedron_fixdeg`. This defines what kind of elements will be used, which determines whether PHAML will be compiled for 2D or 3D problems. See Section 4.4 for the difference between `tetrahedron` and `tetrahedron_fixdeg`.
- `PHAML_GRAPHICS metro mesa none opengl`. This defines what OpenGL library should be used. `opengl` refers to vendor OpenGL libraries, `mesa` to the MESA library, `metro` to a commercial OpenGL library for Linux, and `none` indicates that the graphics program should not be built.
- `PHAML_BLAS atlas compiler goto standard vendor`. This defines the BLAS library to use. `atlas` and `goto` are as mentioned in Section 2.1.3. `compiler` refers to a BLAS library provided with the Fortran compiler defined in `PHAML_F90`. `vendor` refers to a BLAS library supplied by the hardware vendor defined in `PHAML_ARCH`. `standard` refers to a BLAS library in a standard location like `/usr/lib`, and often is not a high performance library.
- `PHAML_LAPACK atlas compiler standard vendor`. This defines the LAPACK library to use, and is usually given the same value as `PHAML_BLAS`.

- `PHAML_SLEPC no yes`. This indicates whether or not to include SLEPc.
- `PHAML_ARPACK no yes`. Should be yes if and only if SLEPc was built with ARPACK support.
- `PHAML_BLOPEX no yes`. Should be yes if and only if SLEPc was built with BLOPEX support.
- `PHAML_PETSC no yes`. This indicates whether or not to include PETSc.
- `PHAML_MUMPS no yes`. Should be yes if and only if PETSc was built with MUMPS support.
- `PHAML_SUPERLU no yes`. Should be yes if and only if PETSc was built with SUPERLU support.
- `PHAML_HYPRE no yes`. Should be yes if and only if PETSc was built with hypre support.
- `PHAML_ML no yes`. Should be yes if and only if PETSc was built with ML support.
- `PHAML_ZOLTAN no yes`. This indicates whether or not to use Zoltan. When Zoltan was compiled, it may or may not have included support for third party libraries. The next few parameters indicate which of them were built into Zoltan. These must agree exactly with how Zoltan was built, or you will get error messages from the linker.
- `PHAML_PARMETIS no yes`. Should be yes if and only if Zoltan was built with ParMETIS support.
- `PHAML_DRUM no yes`. Should be yes if and only if Zoltan was built with DRUM support.
- `PHAML_SYSTEM none dirac looney pepe raritan suns stampede`. This designates a specific computer system for overriding configuration variables in Step 3. Usually it is the hostname of the system.

If you don't find a value that matches your system, you can either (1) add that value and modify `mkmkfile.sh` to handle it by mimicking what is done for other values, or (2) use a similar value and edit `Makefile` to correct it for your system. However, if you edit `Makefile` then you will lose your changes the next time you run `mkmkfile.sh`.

In step 2, set the paths, library names, etc. Here you set shell variables in `mkmkfile.sh` with the names of commands, flags, paths, library names, etc., for the configurations you will be using. Many of these will already be correct, but examine them because some of them are specific to the systems on which PHAML was developed. In particular, many of the compiler command names have been changed to avoid conflicts between multiple compilers on one system, and nearly all of the paths will vary between systems.

In step 3, you can override values set in step 2 for particular system configurations. For example, suppose your MPI library has a different name on Linux than it has on all your other systems. Then in step 2 you set the name used on most systems, and in step 3 you override it if `PHAML_SYSTEM` is your linux box.

There are two other ways to override the default configuration variable values: 1) on the command line for `mkmkfile.sh` (described below), and 2) by setting environment variables in your shell. If an environment variable exists with the same name as a configuration variable, the value of that environment variable is used. Usually these variables are set in the shell startup file. For csh-type shell, an example is

```
setenv PHAML_OS linux
```

Once you finish modifying `mkmkfile.sh`, running it will create `Makefile` in the `src` directory and all the subdirectories under `example` and `testdir`. If a file named `Makefile` already exists, it is moved to `Makefile.bak` before the new file is created. To accept the default configuration, just run

```
./mkmkfile.sh
```

To override the default values and values given by environment variables, specify them on the command line by giving a space-separated list of configuration variables and values. Here, including the "`PHAML_`" part of the configuration variable is optional. For example,

```
./mkmkfile.sh PARALLEL messpass_spawn PARLIB lam
```

2.2.2 Compiling the Library

Once `Makefile` has been built, just type `make` in either the PHAML root directory or `src` subdirectory to compile the PHAML library. If this shows that `Makefile` has errors in it, you can either edit `Makefile` to fix them (but then they will appear again if you need to run `mkmkfile.sh` again), or fix the errors in `mkmkfile.sh` and rebuild `Makefile`. This will create the PHAML library `libphaml.a` and copy it to subdirectory `lib`. It also copies any module files (e.g., `*.mod`) to subdirectory `modules`, and creates a file `lib/CONFIG` that contains the values of the configuration variables used to create the library.

2.3 Testing the Library

After creating the PHAML library, you can test it by running the PHAML Test Suite. The suite contains over 100 short test programs to test nearly all aspects and options of PHAML. Tests that do not apply to the current compilation of the library are skipped. The tests have not yet been written for `PHAML_PARALLEL=messpass_nospawn` (i.e. SPMD programs). They can only be run with `sequential`, `messpass_spawn`, `openmp` or `hybrid_spawn` programs.

To run the full test suite on an interactive system, enter the command

```
make test
```

from either the PHAML root directory or the `testdir` subdirectory. If you are using a batch system like PBS or Torque/Maui, you can run the tests with one of the PBS scripts in the `testdir` directory. To delete all the files that were created by the tests, enter the command

```
make test what=clean
```

The tests can be grouped into three categories. The first tests consists of two very simple programs to verify that a program can be compiled, linked and run. The interactive tests test the use of the `pause` variables to `phaml_solve_pde`, spawning in a debug window, and graphics. The remaining tests are the noninteractive tests. Depending on how many optional auxiliary packages are included, the speed of your computer system, etc., these may take anywhere from a few minutes to a few hours to run.

You can run just the first tests, just the first and interactive tests, or just the first and noninteractive tests with the commands

```
make test what=first
make test what=interactive
make test what=noninteractive
```

If you are running the tests from a batch system where you cannot respond to interactive prompts, you should use `what=noninteractive`.

The individual interactive tests can be run by giving `what` the value `pause`, `debug`, or `graphics`. The noninteractive tests are in the directories `testdir/test_*`. You can run individual noninteractive tests by giving `what` the name of the subdirectory, with or without `test_`. For example, to run the PETSc tests you can use either

`make test what=test_petsc`, or
`make test what=petsc`

The results of the tests are printed both to the screen and to the file `testdir/testresults`. The file only contains standard output, not standard error, so things like messages from the compiler will not appear in the file. Each test consists of a short program that is compiled and run with the output directed to a file. The file is compared to an existing file that contains the expected output. Each test is identified as SUCCESS, FAILURE or WARNING. WARNING indicates that the output is not the same as the comparison file. Often this difference is just minor numerical differences (accumulated round off error) due to different processors, compilers, versions of auxiliary packages, etc. The warning message will direct you to a file that contains the differences, as identified by `diff`, which you should examine to see if the differences are significant.

2.4 Compiling and Running the Examples

Next you compile your application and link in the PHAML library. With most compilers you will need to specify the location of the module files when compiling program units that `use phaml`. Many compilers use the `-I` flag for this (e.g. `f90 -I $PHAML_HOME/modules myprog.f90`), but you should check your compiler's documentation. You also need to link with the PHAML library (e.g. `f90` `myprog.f90 -L$PHAML_HOME/lib -lphaml`) and any other libraries your program needs (MPI, OpenGL, LAPACK, etc.). Your best start is to look at the examples in the `examples` directory, and their `Makefiles`. These `Makefiles` were created when you ran `mkmkfile.sh` in the top PHAML directory. You should not run the `mkmkfile.sh` in the `examples` subdirectories.

With the examples, a successful `make` will create up to three executables:

1. the primary executable `phaml`. This is the program you run.
2. `phaml_slave` if `PHAML_PARALLEL` is `messpass_spawn`. This is spawned by `phaml`.
3. `phaml_graphics` if `PHAML_GRAPHICS` is not `none` and `PARALLEL` is not `messpass_nospawn`. This is spawned by `phaml` and `phaml_slave` if `PARALLEL` is `messpass_spawn`, or run from the command line if `PARALLEL` is `sequential`.

In the PHAML root directory, `make clean` will remove any files created by compilation (e.g. `*.o`) in `src`, `examples/*`, and `testdir/*`. `make reallyclean` will also remove everything in `lib` and `modules`, and the `Makefiles`.

In general, you run `phaml` as you would any parallel program that uses the message passing library you have selected. Some examples are:

1. A sequential compilation. Run the primary program.

   ```
   phaml
   ```

   If you requested graphics, you must also run the graphics program.

   ```
   phaml_graphics
   ```

2. LAM MPI, with spawning. You only start the master program, which spawns the slaves and graphics, so specify the number of processors to be 1.

   ```
   mpirun -w -np 1 phaml
   ```

   I have also found that in this case you don't need to use `mpirun`, you can just execute the master.

   ```
   phaml
   ```

3. MPICH MPI, as an SPMD program. Since this does not spawn the slaves and graphics, you must use `mpirun` to specify the right number of processes. If there are to be n slaves, this consists of the sum of the following: One for the master, n for the slaves, one if the master is doing graphics, and n if the slaves are doing graphics. For example, if there are four slaves and the master is doing graphics,

   `mpirun -machinefile <`*file with list of hosts*`> -np 6 phaml`

4. For OpenMP or hybrid OpenMP/MPI programs, set the OMP_NUM_THREADS environment variable to the desired number of threads, probably equal to the number of cores on the SMP computer, or number of cores on each node of the distributed memory parallel computer, and run the same as a sequential or MPI program.

5. See also the file `doc/HINTS` for my notes on running under debuggers, using ssh, redirecting displays, etc.

If you request graphics, a window should pop up with the graphical display. The following actions are defined by default:

- arrow keys - pan
- left mouse button - rotate
- middle mouse button - zoom
- right mouse button - a menu of actions

The menu contains a large number of ways to change the graphics. See Section 3.5 for further details.

Chapter 3

Scalar Linear Elliptic Boundary Value Problems

The primary function of PHAML is to solve second-order scalar linear self-adjoint elliptic partial differential equations of the form given in Equation 1.1 with Dirichlet, natural (often Neumann), or mixed boundary conditions given by Equations 1.2 and 1.3. This section explains how to write a program that uses PHAML to solve these problems. Other classes of problems that can be solved using PHAML are addressed in subsequent sections. The information here is organized by concept. For an organization by subroutine and parameters, see the reference guide in Section 6.

3.1 Main program

PHAML is a library of subroutines. The user must write a program that calls these subroutines to solve the application problem. Ordinarily this just requires a simple main program and subroutines that define the equations, but the program can be as complex as needed. Subroutines in the PHAML library can be called from either the main program or subroutines.

3.1.1 Parallelism

There are six models of parallel processing supported by PHAML. The programming model used must correspond to the one specified by `PHAML_PARALLEL` in `mkmkfile.sh` when the PHAML library was built (see Section 2.2.1). The correspondence is given in Table 3.1.

In the master/slave model, the parallelism is almost transparent to the user. The user only needs to specify `nproc` in `phaml_create`, and start the program in the manner specified by the message passing library, requesting 1 process. With some libraries, for example LAM and MPICH2, even this can be transparent,

model	PHAML_PARALLEL
sequential	`sequential`
master/slave	`messpass_spawn`
SPMD	`messpass_nospawn`
OpenMP SMP	`openmp`
hybrid OpenMP/MPI master/slave	`hybrid_spawn`
hybrid OpenMP/MPI SPMD	`hybrid_nospawn`

Table 3.1: Correspondence between `PHAML_PARALLEL` in `mkmkfile.sh` and the parallel programming model.

since you can just run the executable when you are only starting 1 process, unless your system uses a queuing program like PBS. Sequential programs can use the same program as a master/slave program, and `nproc` will be ignored. Single Program Multiple Data (SPMD) programs require a little more knowledge of the parallelism. Each instance of the program must determine if it is to be the master, a slave, or a graphics server, and act accordingly. This is explained in the next section. Since SPMD PHAML programs behave as if they were a master/slave program, with process 0 acting as the master, this document will often make reference to the master and slaves, even though the program might be SPMD. With OpenMP, the parallelism is completely transparent to the user, except for setting the desired number of threads for each process through the environment variable OMP_NUM_THREADS or the `nthread` argument to `phaml_create`. Usually this is equal to the number of cores on an SMP computer, or, for hybrid OpenMP/MPI programs, the number of cores on each node of a distributed memory parallel computer or cluster. However, it is sometimes advantageous to use one less than the number of cores if the operating system is running a lot of background processes that would run on the unused core.

3.1.2 Program structure

3.1.2.1 Master/slave and Sequential

In a master/slave program, the user writes a program for the master process. The same program can be used for sequential, OpenMP and hybrid OpenMP/MPI master/slave models. The slave and graphics programs are given in the `src` directory as `slave.f90` and `graphmain.f90`. To compile these programs, see the `Makefile`s in the `examples` directory.

Figure 3.1 illustrates a very simple main program for a master/slave model. More complicated examples can be found in the `examples` directory. This example illustrates the main steps in writing a PHAML program.

First it must use module `phaml`. This gives access to all the public subroutines, the defined constants that are used as values for subroutine arguments, the `phaml_solution_type` data structure, and the defined constant `my_real` which contains the kind number for reals in PHAML.

```
program simple
use phaml
type(phaml_solution_type) :: sol
call phaml_create(sol,nproc=2)
call phaml_solve_pde(sol,                          &
                     max_vert=100000,              &
                     print_grid_when=PHASES,       &
                     print_grid_who=MASTER,        &
                     print_error_when=PHASES,      &
                     print_Linf_norm_error=.true., &
                     print_error_who=MASTER)
call phaml_destroy(sol)
end program simple
```

Figure 3.1: A simple main program.

Second, there must be at least one variable of type `phaml_solution_type`. Variables of this type contain all the information known about the solution of the equation, including the current grid, solution, parallel processes, etc. The type is a public entity in module `phaml`, but the internals of the type are private. This means you cannot directly manipulate components of the variable, you can only pass it to the PHAML subroutines that operate on it.

Next, the solution variable is initialized by subroutine `phaml_create`. This creates an initial grid, allocates and initializes other components of the variable, and, for master/slave programs, spawns the slave and graphics processes. Here we requested the use of 2 slave processors. Other arguments will be discussed in subsequent sections as they become relevant. A full list can be found in Section 6.4.4.

The PDE is solved by calling `phaml_solve_pde`. This subroutine requires that the first argument be a solution variable. There are over 100 more arguments to this subroutine, which will be discussed in subsequent sections and can be found in Section 6.4.15. To make this manageable, all arguments are optional, have reasonable defaults, and should be given as keyword arguments, i.e. *dummyarg=value*, as shown in the example.

Finally, the solution variable should be destroyed by `phaml_destroy` to free memory and terminate any processes that were spawned by `phaml_create`.

3.1.2.2 SPMD

An SPMD program is more complicated because the master, slave and graphics processes are identical. However, it still operates like a master/slave program, so each process must determine if it is the master, a slave, or a graphics server. This is illustrated in Figure 3.2 for a program that uses an MPI library. The same program can be used for a hybrid OpenMP/MPI SPMD model.

In addition to using `module phaml`, it must use `module mpif_mod` to get

```
program simple_spmd
use phaml
use mpif_mod
integer :: whodrawg
integer :: jerr
integer :: my_processor, total_nproc
integer :: nslave, subtract, divide

! initialize MPI, find out how many processors and what my rank is

call mpi_init(jerr)
call mpi_comm_size(MPI_COMM_WORLD,total_nproc,jerr)
call mpi_comm_rank(MPI_COMM_WORLD,my_processor,jerr)

! set the graphics options

whodrawg = NO_ONE

! determine how many processors for slaves and graphics

subtract = 1
if (whodrawg == MASTER .or. whodrawg == EVERYONE) subtract = 2
divide = 1
if (whodrawg == SLAVES .or. whodrawg == EVERYONE) divide = 2
nslave = (total_nproc-subtract)/divide

! call the master, slave or graphics program depending on my rank

if (my_processor == 0) then
   call phaml_master(whodrawg,nslave)
elseif (my_processor <= nslave) then
   call phaml_slave
else
   call phaml_graphics
endif
end program simple_spmd

subroutine phaml_master(whodrawg,nslave)
use phaml
integer, intent(in) :: whodrawg, nslave
type(phaml_solution_type) :: sol
call phaml_create(sol,nproc=nslave,draw_grid_who=whodrawg)
call phaml_solve_pde(sol, ... )
call phaml_destroy(sol)
end subroutine phaml_master
```

Figure 3.2: An SPMD main program using MPI.

```
subroutine pdecoefs(x,y,cxx,cxy,cyy,cx,cy,c,rs)
use phaml
real(my_real), intent(in) :: x,y
real(my_real), intent(out), dimension(:,:) :: cxx,cxy,cyy,cx,cy,c
real(my_real), intent(out), dimension(:) :: rs
cxx=1
cxy=0
cyy=1
cx=0
cy=0
c=0
rs=0
end subroutine pdecoefs
```

Figure 3.3: `pdecoefs` for Laplace's equation.

access to the MPI include file.

The first step is to initialize MPI, determine how many processes there are, and determine the rank of this process. This is needed to determine what type of process this will be, so it cannot be hidden inside `phaml_create` like it is for master/slave programs.

Then the number of slaves is computed based on the total number of processes (which is specified when the program is launched, for example by `mpirun`) and how many graphics processes are needed.

Each process determines its type based on its rank (`my_processor`) and the number of slaves, and calls the corresponding main subroutine. The slave and graphics main subroutines are in the PHAML library. The main subroutine for the master is nearly identical to the main program in the master/slave model, as shown in Figure 3.2.

3.2 Defining the problem

3.2.1 Defining the PDE

The PDE in Equation 1.1 must be defined in subroutine `pdecoefs`. For convenience, the equation is repeated here.

$$-\frac{\partial}{\partial x}\left(c_{xx}\frac{\partial u}{\partial x}\right)-\frac{\partial}{\partial x}\left(c_{xy}\frac{\partial u}{\partial y}\right)-\frac{\partial}{\partial y}\left(c_{yy}\frac{\partial u}{\partial y}\right)+c_x\frac{\partial u}{\partial x}+c_y\frac{\partial u}{\partial y}+c_u u=f \quad \text{in } \Omega$$

`pdecoefs` receives a point (x, y) and returns the value of the functions c_{xx}, c_{xy}, c_{yy}, c_x, c_y, c_u and f at that point in the arguments `cxx`, `cxy`, `cyy`, `cx`, `cy`, `c` and `rs` respectively. The interface for this routine is given in Section 6.3.6. For a scalar PDE, the return variables are 1×1 arrays (they have higher dimension for systems of equations; see Section 4.2) and can be assigned with a whole array assignment statement, making their "arrayness" transparent. Figure 3.3 shows how `pdecoefs` could be written for Laplace's equation $\nabla^2 u = 0$.

Certain characteristics of the PDE might have an effect on the solvers. For example, if there are first order terms then the matrix is not symmetric and a nonsymmetric solver must be used. Also, PHAML can take advantage of some characteristics, such as knowing the operator is the Laplacian, to get better performance. PHAML attempts to determine the relevant characteristics by sampling `pdecoefs` at the midpoints of the initial grid. It is possible for this test to fail. If so, you can force PHAML to know the characteristic through the following arguments to `phaml_solve_pde`:

- Set `pde_has_first_order_terms` to `.true.` if c_x or c_y is not identically zero.
- Set `pde_has_cross_derivative` to `.true.` if c_{xy} is not identically zero.
- Set `laplacian_operator` to `.true.` if c_{xx} and c_{yy} are identically one while c_{xy}, c_x, c_y and c are identically zero.
- Set `isosceles_right_triangles` to `.true.` if every initial element is an isosceles right triangle and they are paired up such that all the right angles are peaks.

In most cases where `task=SET_INITIAL` the automatic testing for these characteristics will call `pdecoefs` before the old solution has been set by `phaml_copy_soln_to_old` resulting in many warnings. You should include the above variables in that call to avoid these warnings.

3.2.2 Defining the boundary conditions

The boundary conditions are defined in subroutine `bconds`. The interface for this routine is given in Section 6.3.1. On each piece of the boundary (Section 3.2.3 explains how to define the boundary piecewise and send a piece ID number to `bconds`) the boundary can be Dirichlet as defined by Equation 1.2

$$u = g,$$

natural (usually Neumann) or mixed as defined by Equation 1.3

$$\left(c_{xx}\frac{\partial u}{\partial x} + c_{xy}\frac{\partial u}{\partial y}\right)\frac{\partial y}{\partial s} - c_{yy}\frac{\partial u}{\partial y}\frac{\partial x}{\partial s} + c_{bc}u = g$$

or periodic (usually on opposite sides of a rectangle).

`bconds` receives as input a point (x, y) at which to return the boundary conditions, and `bmark`, an integer ID number for the piece of the boundary that (x, y) is on. This ID is defined along with the boundary of the domain (Section 3.2.3).

```
subroutine bconds(x,y,bmark,itype,c,rs)
use phaml
real(my_real), intent(in) :: x,y
integer, intent(in) :: bmark
integer, intent(out) :: itype
real(my_real), intent(out) :: c(:,:),rs(:)
if (bmark == 1) then
   itype = NATURAL
else
   itype = DIRICHLET
endif
c=0
rs=0
end subroutine bconds
```

Figure 3.4: `bconds` for homogeneous boundary conditions, natural on boundary piece 1 and Dirichlet elsewhere.

boundary condition	`itype`
Eq. 1.2	`DIRICHLET`
Eq. 1.3 with $c_{bc} = 0$	`NATURAL`
Eq. 1.3 with $c_{bc} \neq 0$	`MIXED`
periodic	`PERIODIC`

Table 3.2: Permitted values for `itype` to specify the type of boundary conditions.

The type of boundary condition for the indicated piece is returned in `itype` using a symbolic constant listed in Table 3.2. The functions c_{xx}, c_{xy} and c_{yy} in Equation 1.3 are the same as those in the PDE, Equation 1.1, which are defined in subroutine `pdecoefs` (Section 3.2.1) and not repeated here. The function c_{bc} in Equation 1.3 is returned in the variable `c`. Finally, the function g in Equations 1.2 and 1.3 is returned in `rs`.

`c` and `rs` are arrays, but for scalar problems the dimensions are all 1, and they can be assigned with a whole array assignment statement. (They have higher dimension for systems of equations; see Section 4.2.)

Assuming the domain is the unit square with the left side assigned 1 for the ID, Figure 3.4 shows a subroutine for the boundary conditions

$$\partial u/\partial n = 0 \quad \text{on} \quad x = 0 \tag{3.1}$$

$$u = 0 \quad \text{elsewhere} \tag{3.2}$$

Periodic boundary conditions say that the value of the solution on one piece of the boundary is the same as the value on another piece. Usually the two pieces are opposite sides of a rectangle, but for generality we need a means of indicating which two pieces are matched up. This is done by making the piece ID of the two pieces have the same absolute value, with one positive and the other negative. `c` and `rs` are not used with periodic boundary conditions, but it is prudent to set them to 0. For an example of periodic boundary conditions, see `examples/periodic`.

Natural and periodic boundary conditions require that there be at least one point with Dirichlet boundary conditions to make the solution unique.

3.2.3 Defining the domain and initial grid

The domain and initial grid can be defined in one of two ways. The first is to supply subroutines that define the boundary explicitly as a piecewise curve in R^2. This approach is required if the boundary is not polygonal, i.e. if it has curved pieces, but can also be used for polygonal domains. The second is to provide triangle data files that were produced by the program Triangle [42]. These files can be created by writing a `.poly` file and running Triangle, or by using the first approach once and saving the triangle data files that PHAML creates, or by using the triangle data files from one of the PHAML examples. In either case, this gives a starting triangulation, which is preprocessed to create the initial grid.

To define the domain with subroutines, you must write three subroutines similar to those used by the domain processor of Rice [40].

`subroutine boundary_point(ipiece,s,x,y)` contains the definition of the boundary. Each piece of the boundary is given by a parametric curve $(x(s), y(s))$ for s in some range of R. The ending point of one piece must be the same as the starting point of the next piece, including the last piece of the outer boundary connecting to the first piece of the outer boundary, and the last piece of each hole connecting to the first piece of the same hole. The input parameters `ipiece` and `s` indicate which piece of the boundary and parameter value to evaluate, and the output parameters `x` and `y` are the requested point on the boundary.

`ipiece` is also used as the boundary marker for the triangle data files, and will be passed to `bcond` (Section 6.3.1) to simplify evaluation of boundary conditions. The endpoints of the boundary pieces will always be vertices of the grid, and are assigned the boundary marker of the piece they start. To get a boundary marker that is unique to an individual vertex, define a boundary piece of length 0 at that vertex (i.e., starting and ending parameters are the same). The last boundary piece cannot be a single point. Instead, make that point be the first piece.

`function boundary_npiece(hole)` (Section 6.3.3) returns the number of pieces used to define the boundary. If hole is 0, it should return the number of pieces that define the outer boundary. Otherwise it should return the number of pieces that define the `hole`th hole. The holes are numbered consecutively starting with 1. boundary_npiece(0) must return a positive integer if and only if subroutines are used to define the boundary. If it returns 0 or a negative integer, the starting triangulation is read from triangle data files. If hole is larger than the number of holes in the domain, it should return 0.

`subroutine boundary_param(start,finish)` returns the range of parameter values for every piece of the boundary. The output variables `start` and `finish` are `real(my_real)` arrays of length equal to the total number of boundary pieces, and should be assigned the starting and ending parameters of each piece.

The starting grid is created by PHAML by creating a `.poly` file for input to Triangle, which is then run to create triangle data files. Running Triangle involves a call to the intrinsic subroutine `system`, which is not standard in Fortran 90. Most compilers provide this routine as an extension, and use the same behavior for it, but if you have trouble you may have to change the definition of `my_system` in `sysdep.f90`.

You can control the fineness of the starting grid with the parameter `max_blen` in `phaml_create`. No triangle boundary side in the starting triangulation will have length longer than `max_blen`, and Triangle is run with `-a max_blen`$^2\sqrt{3}/4$ to limit the area of the triangles to that of an equilateral triangle with side length `max_blen`.

The name of the `.poly` file is determined by the parameter `triangle_files` in `phaml_create`, which has the default value `"domain"`. The file name will be the character string with the added suffix `.poly`. Note that if the full path is not given in `triangle_files`, the location of the file may be compiler dependent. If PHAML is run MPI parallel, the file must be placed on a file system that is shared by all the processes, which may require specifying the full path.

The second method for defining the domain and initial grid is to use triangle data files. These are the edge (`.edge`), element (`.ele`), neighbor (`.neigh`), node (`.node`) and poly (`.poly`) files created by the program Triangle.

To indicate that the starting grid is given by triangle data files, have `function boundary_npiece(0)` return 0 or a negative number. The parameter `triangle_files` in `phaml_create`, which has the default value `"domain"`, then contains the root of the name of the five triangle data files. If Triangle inserted an iteration number (e.g. `.1`) into the name, then it should be included.

If you are solving a PDE on the unit square, or on one of the other domains in the examples, then you only need to copy the triangle data files from the example and, if necessary, specify the name of the files.

Otherwise you must define the polygonal domain with a `.poly` file, which is basically a list of vertices and boundary line segments. Holes are allowed. See the documentation for Triangle [43] for the exact definition of a `.poly` file. You should specify a boundary marker for each vertex and boundary segment. The boundary marker must be 0 if and only if the vertex or edge is interior, i.e., not on the boundary. This boundary marker will be passed to function `bcond` to simplify the definition of boundary conditions. With a `.poly` file defined, create the triangle data files with the command

```
triangle -pneqj root_of_filename.poly
```

The `-p` flag indicates the input is a poly file. The `-n`, and `-e` flags force the writing of neighbor and edge files. The `-q` flag requests a quality mesh, which imposes bounds on the angles. The `-j` flag says to jettison (remove) vertices that are not part of the triangulation. Also, the `-a` flag may be useful to impose a maximum size (area) of the triangles, and the `-I` flag can be used to prevent the insertion of the iteration number in the filename. See the documentation for Triangle [43].

Regardless of whether they are created by Triangle from a `.poly` file, created by PHAML from the boundary subroutines, or copied from somewhere else, the triangle data files define a starting triangulation. PHAML requires an initial grid that satisfies certain conditions. This initial grid is determined from the starting triangulation automatically by PHAML through a process of refinement and grid smoothing. The triangles of the initial grid are obtained by bisection or trisection of the starting triangles, followed by some node movement.

3.2.4 The true solution

If the true (a.k.a. exact or analytical) solution is known, it and its first derivatives can be provided through subroutines `trues`, `truexs` and `trueys`. If these are provided, then the program can print norms of the error (Section 3.4.2) or choose the error as the function to visualize with the graphics. If `trues` is defined, but `truexs` and/or `trueys` is not, then the energy norm, H^1 norm, and H^1 semi-norm of the error cannot be printed, but all other norms and the graphics are still valid.

The interfaces for these routines are given in Sections 6.3.9, 6.3.10 and 6.3.11. They are function subroutines that return the value of the solution, x derivative of the solution, and y derivative of the solution, respectively. The input variables give the point (x, y) at which to return the solution. There are also two input variables, `comp` and `eigen`, that are not relevant for scalar boundary value problems (they are used for systems of equations and eigenvalue problems).

3.3 Solution method

There are many arguments to `phaml_solve_pde` that affect the details of the solution method. This section explains the options available. It is organized with sections on discretization, refinement, the error indicator, the linear system solver, load balancing and termination. Each section briefly describes the methods used, but this is not intended to be a thorough treatment of parallel adaptive multilevel finite element methods. See the references for more details of the methods.

See also Section 6.4.15 which formally defines the arguments to `phaml_solve_pde`.

3.3.1 Discretization

PHAML uses a standard Galerkin finite element method (see, for example [45][47]) to approximate the solution of Equations 1.1-1.3, which we briefly describe here. The domain is partitioned into a set of conforming triangles, T, (the grid or mesh) and the approximation space is defined as the Hilbert space of continuous functions that are polynomials over each triangle. The degree of the polynomial can be different over different triangles. The p-hierarchical basis, $\Phi = \{\phi_i\}$, of either Szabo & Babuška [47] or Carnevali et al. [12] spans the space, and gives a representation for the approximate solution

$$u_T = \sum_{\phi_i \in \Phi} \alpha_i \phi_i \tag{3.3}$$

Basis functions can be categorized in three groups. The linear ($p = 1$) basis functions are in one-to-one correspondence with the vertices of the grid. Higher order basis functions are associated with edges or faces (triangles). There are $p - 1$ edge bases associated with an edge of degree p, and $(p - 1)(p - 2)/2$ face bases associated with a face of degree p.

The space has the energy inner product defined by

$$\langle u, v\rangle = \int_\Omega c_{xx}u_x v_x + c_{xy}u_y v_x + c_{yy}u_y v_y + c_x u_x v + c_y u_y + c_u uv \tag{3.4}$$

where c_{xx}, c_{xy}, c_{yy}, c_x, c_y, and c_u are from Equation 1.1, and the subordinate energy norm $\|u\|^2 = \langle u, u\rangle$. (Note: We need $c_{xy} = c_x = c_y = 0$ for 3.4 to be an inner product because of symmetry, and $c_u \geq 0$ for $\langle u, u\rangle$ to be a norm because of positivity, but formally we proceed with these definitions knowing that some of the following statements are not strictly true.) The approximate solution is the function in the space that minimizes the energy norm of the error, i.e. the error is orthogonal to the space under the energy inner product. Thus the approximate solution satisfies

$$\langle u_T, \phi_i\rangle = \langle f, \phi_i\rangle_2 \quad \forall\phi_i \in \Phi \tag{3.5}$$

where $\langle ., .\rangle_2$ is the L_2 inner product $\langle u, v\rangle_2 = \int_\Omega uv$. Substituting Equation 3.3 into Equation 3.5 leads to the discretized form of the problem $Ax = b$

with $a_{ij} = \langle \phi_i, \phi_j \rangle$, $b_i = \langle f, \phi_i \rangle_2$, and x the vector of α_i's. Natural boundary conditions are imposed automatically by the energy inner product. Dirichlet boundary conditions are imposed by replacing the corresponding equations with equations that set the corresponding α_i's directly from the boundary condition.

Also of interest is the H^1 norm

$$||u||_{H^1} = \int_\Omega u_x^2 + u_y^2 + u^2 \tag{3.6}$$

and H^1 semi-norm

$$|u|_{H^1} = \int_\Omega u_x^2 + u_y^2 \tag{3.7}$$

There are only six arguments that affect how discretization is performed. First, you can select the degree of the polynomials in the approximation space with the argument `degree`. This sets all elements to start with the given degree, even if you use *p*- or *hp*-refinement. Second, the integrals of Equation 3.4 are computed by numerical quadrature, with the order of the quadrature rule determined such that integrals are exact for polynomials of the degree $2(p-1)$ where p is the degree of the basis over each triangle. Sometimes this may not be accurate enough, in which case you can supply an increase of the order through `inc_quad_order`. Third, in triangles that are owned by a different processor (see Section 3.3.5), the quadrature is performed by the owner and communicated by message passing. If this were not done, then the integrals over those triangles would be less accurate than the same integrals on the processor that owns the triangle, because it will have refined the triangle into many smaller triangles. However, sometimes this doesn't matter, such as when solving Laplace's equation (all the integrals are exact) or when using a solver other than the (default) hierarchical basis multigrid solver 3.3.4.1, which don't use the unowned triangles. You can avoid the extra computation and communication with `ignore_quad_err=.true.` Next, by default PHAML does not put any limitation on how much the degrees of neighboring elements can differ. You can control this through `p_compatibility`, which has a default of `PCOMPAT_NONE`, and `max_p_diff`, which has a default of 1. If you use `PCOMPAT_INCREASE`, and the degrees of two neighboring elements differ by more than `max_p_diff`, then the one with smaller degree is increased to $p-$`max_p_diff`, where p is the larger degree. Similarly, `PCOMPAT_DECREASE` causes the larger value to be decreased to enforce compatibility. However, use of `PCOMPAT_DECREASE` is discouraged because it can cause refinement to stall. Finally, you can select how the degree of an edge is determined when the triangles that share that edge have different degrees through `edge_rule`. If you select `MINIMUM_RULE` (the default), then the edge gets the smaller of the two triangle degrees. If you select `MAXIMUM_RULE`, then the edge gets the larger of the two triangle degrees.

3.3.2 Refinement

One of the major phases in `phaml_solve_pde` is refinement of the grid to increase the size of the approximation space, which reduces the norm of the discretization

`DOUBLE_NVERT`
`DOUBLE_NELEM`
`DOUBLE_NEQ`
`HALVE_ERREST`
`KEEP_NVERT`
`KEEP_NELEM`
`KEEP_NEQ`
`ONE_REF`
`ONE_REF_HALF_ERRIND`
`MATCH_TOL`

Table 3.3: Permitted values for `refterm` to determine how much refinement to do.

error. h-refinement refers to subdividing triangles by newest node bisection (see [29] [31] for 2D, and [6] for 3D). p-refinement refers to increasing the polynomial degree over a triangle. In either case the refinement can be undone, referred to as derefinement or coarsening. Derefinement can be switched off with the argument `derefine=.false.` Refinement can be done uniformly, i.e. refine all triangles in the grid, or adaptively, i.e. refine a selected subset of the triangles.

The type of refinement that is performed is determined by the argument `reftype`. This argument can have one of the values `H_UNIFORM`, `H_ADAPTIVE`, `P_UNIFORM`, `P_ADAPTIVE` or `HP_ADAPTIVE`. With `HP_ADAPTIVE` an element may be refined by either h- or p-refinement. hp-adaptive strategies are explained later in this section.

With h-adaptive and p-adaptive refinement, the refinement phase consists of a coarsen-refine loop. At the beginning of each time through the loop, a coarsen cutoff and refine cutoff is determined, and elements are marked for coarsening or refining. In general, an element is marked to be coarsened if its error indicator (Section 3.3.3) is less than the coarsen cutoff, and marked to be refined if its error indicator is greater than the refine cutoff. However, some elements are not coarsenable or refinable. An element is not h-coarsenable if it is in the initial grid, it or any of its siblings (the children of the parent and the parent's mate) has children, or any of its siblings have an error estimate larger than the coarsen cutoff. Also, it will not be coarsened if it has already been coarsened and then the parent rerefined within this refinement phase, to prevent an infinite loop (but see an exception under MATCH_TOL below). An element cannot be p-coarsened if it has degree 1. An element cannot be h-refined if the level of the children would exceed `max_lev` or the size of the children would be smaller than `min_elem_size`, and cannot be p-refined if its degree would exceed `max_deg`.

The cutoffs are determined by the arguments `coarsentol`, `reftol`, `coarsentol_factor`, `reftol_factor`, and `reftol_scale_energy`. If `coarsentol` is given as a positive real number, the coarsen cutoff is `coarsentol/coarsentol_factor`, and if `reftol` is given as a positive real number, the refine cutoff is `reftol/reftol_factor`.

There are also some special values for `coarsentol` and `reftol`. If `reftol` is `MAX_ERRIND_OVER_FACTOR`, the refine cutoff is the maximum error indicator (over all refinable elements) divided by `reftol_factor`, and likewise for `coarsentol`. If `coarsentol` is `REFCUTOFF_OVER_FACTOR`, the coarsen cutoff is the refine cutoff divided by `coarsen_factor`. If `coarsentol` is `REFCUTOFF_TIMES_CONVERGENCE`, the coarsen cutoff is the refine cutoff divided by `coarsen_factor` and multiplied by the energy norm asymptotic convergence rate, $(1/2)^{p/2}$ where p is the degree of the element. If `reftol_scale_energy` is `.true.`, the refine cutoff is divided by the square root of the number of elements, and if in addition `errtype` is `RELATIVE_ERROR`, the refine cutoff is multiplied by the energy norm of the computed solution. (See `ONE_REF` below.)

Each time through the coarsen-refine loop, first all elements marked for coarsening are coarsened, in order of finest level to coarsest level, and then all elements marked for refinement are refined, going from coarsest level to finest level.

There are several ways to determine how much refinement to perform in one refinement phase, i.e., when to exit the coarsen-refine loop. This is controlled by the argument `refterm`. The allowed values for this argument are given in Table 3.3. Under any of these choices the coarsen-refine loop is also exited after going through it `refmaxloop` times. This limit prevents an infinite loop if coarsening and refining negate each other.

"Double" means that the refinement should approximately double the number of vertices, elements or equations in the grid. The factor 2 was chosen because this corresponds to the increase that would occur with one uniform h-refinement of the grid. If a different factor is desired, it can be specified with the real valued argument `inc_factor`. The number of the specified entities is not doubled exactly because all elements marked for refinement are refined. The coarsen-refine loop is exited when the number of elements is a least doubled.

"Keep" attempts to change the grid by derefining some elements and refining others while keeping the total number of entities approximately the same. This is useful, for example, with time dependent problems where the grid should track the movement of some feature of the solution. If the corresponding "max_" value is supplied (for example, `max_vert` along with KEEP_NVERT), then the attempt is to match the number supplied. Otherwise, the attempt is to match the number of entities currently in the grid, which can cause a drift in the number of entities after several iterations.

`HALVE_ERREST` refines the grid until the maximum error indicator has been reduced by half. This corresponds to the expected reduction of error by a uniform h-refinement with `degree=1` and a smooth solution.

With `ONE_REF` the coarsen-refine loop is exited after one repetition. The default refinement parameters with this choice are `reftol=term_energy_err` (Section 3.3.6), `reftol_factor=1.0` and `reftol_scale_energy=.true.` Using this, if the error indicator of every element is exactly refine cutoff, the global energy norm error estimate is exactly `term_energy_err`.

`ONE_REF_HALF_ERRIND` is like `ONE_REF` except the default refine parameters are `reftol=MAX_ERRIND_OVER_FACTOR`, `reftol_factor=inc_factor` and `reftol_` scale_energy=.false., so this makes one pass refining elements with error indicators larger than half the maximum.

MATCH_TOL repeats the coarsen-refine loop until the error indicator of all elements is between the coarsen cutoff and refine cutoff, except those that are not coarsenable or refinable. For this the cutoffs are computed the first time through the coarsen-refine loop, and remain constant thereafter. Normally the ban on coarsening an element that was already coarsened and then recreated by the parent being refined is reset at the beginning of the coarsen-refine loop. With MATCH_TOL it is possible for this to result in an infinite refine-solve loop by having the refinement negate the coarsening, giving the same grid back after the refinement phase. To avoid this, the reset is not performed after the recoarsen_limitth time through the refine-solve loop if the change in the number of elements in the previous refinement phase was less than recoarsen_tol times the number of elements in the grid.

A large number of strategies for *hp*-adaptive refinement have been implemented in PHAML. Selection of which strategy to use is controlled by the argument hp_strategy. Some strategies may override the values of some arguments, in particular refterm, derefine, inc_factor, and error_estimator. The strategies are briefly described here. For a more complete description, see [35, 36]. For a comparison of how the different strategies performed on a set of test problems, see [36, 37].

In all of the *hp* strategies, if an element that would be refined by p refinement has degree max_deg, then it is refined by h refinement (unless stop_on_maxdeg is true), and if an element that would be refined by h refinement has level max_lev or size less than min_elem_size, then it is refined by p refinement (unless the level is max_lev and stop_on_maxlev is true). If an element has both max_deg and max_lev or min_elem_size, then it is not refined.

The following values are currently allowed for hp_strategy:

HP_APRIORI is an extension of the second strategy in Ainsworth & Senior [2]. The basic approach is to refine elements by p refinement, except elements that contain a known point singularity are refined by h refinement. The extension is that we do not limit irregularities to point singularities, and you can specify the strength of that irregularity.

This strategy requires that the user provide a function subroutine that indicates where the solution has an irregularity (i.e. is singular or nonsmooth). See the end of examples/L-domain/pde.f90 for an example of this subroutine. Also see Section 6.3.8. In theory, this routine should return the largest value of m such that the solution is in $H^m(T)$, i.e. the derivative up to order m are in L^2, where T is the triangle whose vertices are given as input to the function. For multicomponent solutions, it should return the worst (i.e. smallest) such m among the components.

In practice, it can be used to guide refinement in other *a priori* known trouble areas, such as sharp peaks, boundary layers and wave fronts. The actual use is that p refinement is performed if the current degree of the triangle is less than the returned value, and h refinement is performed otherwise. So, for example, if you know some region contains a boundary layer, you could return 3.1 for any triangle that intersects that region to perform h-refinement with cubic elements over the boundary layer.

Several hp-adaptive strategies use the same principle as the `HP_APRIORI` strategy, but attempt to estimate the regularity in various ways. `HP_NEXT3P` is an implementation of the first strategy given in Ainsworth & Senior [2]. Three error estimates are computed by the equilibrated residual method with spaces of degree $p+1$, $p+2$ and $p+3$, where p is the current degree of the element. If ϕ is the actual error over the element, the error estimates η_{p+q}, $q=1,2,3$, converge to ϕ with error bounds

$$||\phi||^2 - \eta_{p+q}^2 \leq C(p+q)^{-2\alpha}.$$

The three error estimates are used to determine the three unknown constants $||\phi||$, C and α. The regularity is then given by $m = 1+\alpha$.

`HP_PRIOR2P_E` and `HP_PRIOR2P_H1` are inspired by a strategy of Suli, Houston and Schwab [46]. Two error estimates are computed using the local p error estimator with spaces of degree $p-1$ and $p-2$. The regularity is estimated by

$$m = 1 - \frac{log(\eta_{p-1}/\eta_{p-2})}{log((p-1)/(p-2))}$$

`HP_PRIOR2P_E` uses the energy norm of the error estimate, whereas `HP_PRIOR2P_H1` uses the H^1 norm.

`HP_TYPEPARAM` selects the type parameter strategy of Gui and Babuška [21]. Perceived smoothness of the solution over element t is given by

$$R(t) = \begin{cases} \frac{e(t,p)}{e(t,p-1)} & e(t,p-1) \neq 0 \\ 0 & e(t,p-1) = 0 \end{cases}$$

where p is the degree of the element and e is the error indicator for the given degree. The type parameter, γ, determines the type of the element. If $R(t) > \gamma$ then t is of h-type and will be h refined; otherwise it is p-type and will be p refined. γ is specified with `tp_gamma`.

Another way of determining if the solution is smooth is to compare the local *a posteriori* error estimate with a prediction of what the error estimate should be, after refinement, under the assumption that the solution is smooth and has the proper asymptotic convergence rate [28]. If η_E is the error estimate on element E, and E' is a child of E after refinement, then the predicted error indicator for E' is

$$\eta_{E'}^{\text{pred}} = \begin{cases} \frac{1}{2}\gamma_h \left(\frac{1}{\sqrt{2}}\right)^{p_E} \eta_E & \text{if } E \text{ was } h \text{ refined} \\ \sqrt{\gamma_p}\eta_E & \text{if } E \text{ was } p \text{ refined} \end{cases}$$

where p_E is the degree of element E, and γ_h and γ_p are control parameters given in `sp_gamma_h` and `sp_gamma_p`. Then, if E' is selected for refinement, it is refined by h-refinement if $\eta_{E'} > \eta_{E'}^{\text{pred}}$, and by p-refinement otherwise. This strategy is selected with `HP_SMOOTH_PRED`.

HP_BIGGER_ERRIND selects a strategy in which both the LOCAL_PROBLEM_H and LOCAL_PROBLEM_P error indicators are computed. It is similar to the strategy for 1D problems in [41]. The error indicator specified by error_estimator is used to determine which elements will be refined (see 3.3.3). For each element that is selected for refinement, it is h refined if LOCAL_PROBLEM_H gives the larger error indicator, and p refined if LOCAL_PROBLEM_P is larger. The premise is that the local problem error indicators approximate how much the solution will change if the refinement is performed, and one should perform the type of refinement that will cause the largest change, and hence reduce the error the most. Experiments have indicated that it is often beneficial to bias the refinement towards p-refinement, which can be done by setting pbias to a number greater than 1. We have found that generally pbias=2 works best if the solution is singular or has exceptionally strong features, and pbias=4 is best for smooth solutions or moderately strong features.

HP_PATCH selects a strategy based on solving local problems on patches of elements that was proposed by Bürg and Dörfler in [10]. The patch consists of the element to be refined, K, and all elements that share an edge with it. We solve the residual problem, like in the local problem error indicators, using homogeneous Dirichlet boundary conditions. Two or more candidate refinements are considered. For candidate j, the patch is refined as indicated by the candidate, the residual problem is solved, and the energy norm of the solution is computed to get $\beta_{K,j}$. $w_{K,j}$ is the number of degrees of freedom in the refined patch. The candidate with the smallest value of $\beta_{K,j}/w_{K,j}$ is selected.

Candidates are defined by two arrays, hp_patch_mult and hp_patch_add, with dimension (2,number of candidates). If p is the current degree of element K, then for the j^{th} candidate, the degree of the i^{th} child of h-refinement, $i = 1, 2$, is $\max(1, \lfloor p * \texttt{hp\_patch\_mult(i,j)} \rfloor + \texttt{hp\_patch\_add(i,j)})$. For example, to consider child degrees $(p/2 + 1, p/2)$ use hp_patch_mult(:,j)=(/.5,.5/) and hp_patch_add(:,j)=(/1,0/). To keep symmetry in the candidates, also include candidate $(p/2, p/2 + 1)$.

The special case where the second entry in hp_patch_mult is zero designates p-refinement. The first entry of hp_patch_mult is ignored and the first entry of hp_patch_add designates how much to increase p. For example, hp_patch_mult(:,j)=(/1.0,0.0/) and hp_patch_add(:,j)=(/2,0/) indicates a candidate p-refinement with p increased by 2.

There are also some defined constants for hp_patch_add to specify special candidate sets. In this case, hp_patch_mult is ignored, if present.

- HP_PATCH_H_P_CANDIDATES indicates the usual two candidates: 1) h-refinement keeping the same p, and 2) p-refinement increasing p by 1. This is the default.

- HP_PATCH_REFSOLN_ELEM_CANDIDATES indicates the candidates used by the HP_REFSOLN_ELEM strategy (defined below): nine h-refinement candidates with degrees $(p_0 + i, p_0 + j)$, $0 \leq i, j \leq 2$, where $p_0 = \lfloor (p + 1)/\sqrt{2} \rfloor$, and two p-refinement candidates increasing p by 1 and 2.

- `HP_PATCH_REFSOLN_EDGE_CANDIDATES` indicates the candidates used by the `HP_REFSOLN_EDGE` strategy (defined below): p h-refinement candidates with degrees (1,p), (2,p-1), (3,p-2), ..., (p,1), and one p-refinement candidate increasing the degree by 1.

A strategy for 1D problems based on the coefficients of the Legendre polynomial expansion of the solution was given in [27]. If p refinement is optimal, then the coefficients should decrease exponentially. A least squares fit of the last four coefficients is made to $ce^{-\sigma p_i}$, where p_i are the degrees of the last four Legendre polynomials. If $\sigma > 1$ then p refinement is performed, otherwise h refinement. To extend this to 2D, we use the coefficients of the p-hierarchical basis. The i^{th} "coefficient" is given by the sum of the absolute values of all coefficients of bases of degree i. This strategy is selected with `HP_COEF_DECAY`.

Another strategy based on Legendre coefficients is given in [22]. This strategy, selected with `HP_COEF_ROOT`, uses a "root test" on the coefficients to estimate the regularity of the solution. p refinement is used where the solution is sufficiently smooth, and h refinement elsewhere. Again, PHAML uses the coefficients of the p-hierarchical basis instead of the Legendre coefficients.

A strategy based on that of Šolín et al. [44] is implemented as `HP_REFSOLN_ELEM`. This strategy has its own overall structure to the adaptive refinement algorithm, so most of the refinement-related parameters to PHAML have no effect, including the error indicator. Also note that the global energy norm error estimate is actually a relative H^1 norm error estimate (which is equivalent), and the L_∞ and L_2 error estimates are not available. However, all the usual error estimates are available through `phaml_query`. The method begins by computing a reference solution, u_{ref} on a grid that has been globally refined by both h and p. The error indicator for element E is computed as $||u_{\text{ref}} - u_T||_{H^1(E)}$. Elements for which the error indicator is larger than the largest error indicator divided by `inc_factor` are selected for refinement. For each element to be refined, 11 candidate refinements are considered: p-refine to degree $p+1$, p-refine to degree $p+2$, and h-refine with the child degrees being all combinations of p_0, p_0+1 and p_0+2 where p is the current degree of the element and $p_0 = \lfloor (p+1)/\sqrt{2} \rfloor$. For each candidate, the H^1 projection of the reference solution onto the corresponding space, $\Pi_{\text{candidate}}$, is computed, and the projection error is computed as $||u_{\text{ref}} - \Pi_{\text{candidate}}||_{H^1(E)}$. The projection error onto the unrefined space is also computed. The winning candidate refinement is selected based on the amount by which the logarithm of the projection error is reduced relative to the increase in the number of degrees of freedom. Experiments have indicated that it is often beneficial to bias the refinement towards p-refinement, which can be done by setting `pbias` to a number greater than 1. We have found that generally `pbias=2` works best if the solution is singular or has exceptionally strong features, and `pbias=4` is best for smooth solutions or moderately strong features. HP_REFSOLN_ELEM has not yet been implemented in parallel, so it currently requires `nproc=1`.

Another strategy based on using a reference solution is that of Demkowicz [13]. HP_REFSOLN_EDGE is based on this strategy. It is similar to

HP_REFSOLN_ELEM, but one first considers the refinement of edges by projecting the reference solution onto spaces corresponding to candidate refinements of the edge. Once it is determined how to refine the edge, the refinement of the element is determined by consistency of the h-refinement of the edge and the minimum edge rule for p. This method has not been implemented in parallel yet, so it currently requires `nproc=1`.

3.3.3 Error indicator

The heart of an adaptive refinement strategy is the error estimator, or more properly, error indicator. An error indicator is computed for each triangle, and those with the largest error indicators are refined. PHAML currently contains six error indicators. The error indicator is selected by the argument `error_estimator` which takes one of the values `EXPLICIT_ERRIND`, `LOCAL_PROBLEM_H`, `LOCAL_PROBLEM_P`, `EQUILIBRATED_RESIDUAL`, `HIERARCHICAL_COEFFICIENT` or `TRUE_DIFF` to select one of the error indicators. It can also take the value `INITIAL_CONDITION`.

Many error indicators are based on the interior residual within elements

$$r = f - \mathcal{L}u_T \tag{3.8}$$

and the boundary residual on element edges

$$R = \begin{cases} g - \mathcal{B}u_T & \text{if the edge is on } \partial\Omega_N \\ 0 & \text{if the edge is on } \partial\Omega_D \\ -[\frac{\partial u_T}{\partial n}] & \text{if the edge is interior} \end{cases} \tag{3.9}$$

where $\mathcal{L}$ is the operator defined in Equation 1.1, $\mathcal{B}$ is the operator defined in Equation 1.3, f, g, $\partial\Omega_N$, and $\partial\Omega_D$ are defined in Equations 1.1-1.3, u_T is the approximate solution, and $[\frac{\partial u_T}{\partial n}]$ is the jump in the normal derivative across the element boundary. See [1] for a more detailed treatment of error indicators.

EXPLICIT_ERRIND selects the explicit error indicator defined in Chapter 2 of [1], with slight modifications for the more general operator and degree-based weights for high order elements as given in [28] . The error indicator is based on the norm of the residual. The explicit error indicator, η_e, for an element e is given by

$$\eta_e^2 = \frac{h_e^2}{p^2}||r||_{L_2(e)} + \frac{h_e}{2p}||R||_{L_2(\partial e)} \tag{3.10}$$

where h_e is the longest edge length of the element and p is the degree of the element. The error indicator is used to guide adaptive refinement. The energy norm error estimate is given by an unknown constant times the square root of the sum of the squares of the error indicators. For the L_2 error estimate, the powers on the h's are increased by 2. For the L_∞ error estimate, the L_∞ norm of the residuals is used and the maximum error indicator gives the error estimate. In PHAML the unknown constant has been chosen to be 1/4 for the energy norm and 1/20 for the L_2 and L_∞ norms based on the results obtained with the example and test problems, although these constants work better with high order or hp-adaptive elements than linear elements. The integrals for the energy and L_2 norms are approximated with a 4th order quadrature rule, and the L_∞ norm is approximated by values at the quadrature points of the same quadrature rule. The H^1 and H^1 semi-norm error estimates are not available when using this error indicator, and will return 0.0. The explicit error indicator is quite efficient to compute and generally provides good guidance for adaptive refinement, but one cannot be certain of the accuracy of the error estimates.

`LOCAL_PROBLEM_H` and `LOCAL_PROBLEM_P` are based on solving a small local problem. Equation 1.1 is modified by replacing f with the interior residual r. For a linear PDE, the solution of this equation is the error. The modified equation is solved on a domain consisting of one or two triangles to get an estimate of the error over that small domain. To approximate the solution of this small problem with slightly higher accuracy than the current solution u_T, the triangle(s) are refined once either by h-refinement or p-refinement. The h-refinement form uses two triangles and refines them as a pair by bisection. Homogeneous Dirichlet boundary conditions are applied. The p-refinement form uses one triangle with polynomial degree one larger than that used for u_T. Natural boundary conditions are applied using the boundary residual R. Since the refinement used for the error indicator is exactly what would occur if the triangle(s) was (were) chosen for refinement by h- or p-refinement, this gives an estimate of how much the solution would change if this triangle(s) was (were) refined. The local problem error indicators are very accurate, but relatively expensive, because of the computation required to set up and solve the elemental matrices for each triangle.

The `EQUILIBRATED_RESIDUAL` error indicator is similar to the `LOCAL_PROBLEM_P` indicator, except that the residual is equilibrated so that the boundary fluxes are in equilibrium with the interior residual loads (see Chapter 6 in [1]). This insures that the discrete Neumann problem has a solution, which in turn allows the use of the full local approximation space of degree p, whereas the `LOCAL_PROBLEM_P` uses a reduced space spanned by the bases of exact degree p. It can be shown that this method produces an error estimate that is a guaranteed upper bound on the actual energy norm of the error, if the local problem was solved exactly. Of course, the local problem is solved approximately so the guarantee does not hold, but the PHAML examples typically find the ratio of error estimate to actual error to be about 1.25. This is the most accurate and stable error indicator in PHAML, but also the most computationally expensive.

A less expensive approach, given by `HIERARCHICAL_COEFFICIENT`, is to simply examine the hierarchical coefficients (see [29]) of u_T over each triangle, which is similar to computing the local problem indicator one refinement back. For linear elements, the coefficient of the h-hierarchical basis is used. For higher order elements, the coefficients of the p-hierarchical bases are used. This indicator can provide a very inexpensive way to guide adaptive refinement, but is not likely to give an accurate estimate of the norm of the error. The H^1 and H^1 semi-norm error estimates are not available when using this error indicator, and will return 0.0.

The `TRUE_DIFF` error indicator uses the difference between the true solution (if given, see 3.2.4) and u_T. The energy, H^1 and L^2 norms, and H^1 semi-norm are estimated with a sixth order quadrature rule, and the L^∞ norm is estimated using the same quadrature points. This is primarily available for comparison with new error indicators and would not normally be used.

The `INITIAL_CONDITION` estimate uses the difference between the function given in subroutine `iconds` and u_T. Normally this is used to define an initial grid for time dependent or nonlinear problems (see Section 4.3), but it can also be used to provide a function that indicates where you believe the grid should be finer.

3.3.4 Linear system solver

Another major phase of `phaml_solve_pde` is the solution of the linear system of equations to get the coefficient vector of the solution. PHAML contains a hierarchical basis multigrid method as the primary linear system solver, along with two basic Krylov space solvers, conjugate gradients and GMRES. It also contains hooks into several freely available software packages of direct and iterative parallel solvers for comparative studies and for situations where the native solvers are not sufficient. For information on obtaining the optional software discussed in this section, see Section 2.1. The solver is selected by the arguments `solver` and `preconditioner`.

3.3.4.1 Hierarchical basis multigrid solver

The default solver is the hierarchical basis multigrid solver (HBMG), which can be explicitly selected with `solver = MG_SOLVER`. (Note: this solver must NOT be used if the linear system is not symmetric (i.e., c_{xy}, c_x or c_y from Equation 1.1 is nonzero, or a coefficient matrix in a coupled system of equations is nonsymmetric) or indefinite (i.e., c_u is negative with sufficiently large magnitude).) It combines the ideas of an *hp*-multigrid method [34] with the h-hierarchical basis multigrid method for linear elements [30]. The equations corresponding to high order face basis functions 3.3.1 are first removed by static condensation [51]. A p-multigrid cycle is applied to the equations corresponding to vertex and edge basis functions as follows. The cycle is like a normal multigrid V-cycle, except the levels are given by the polynomial degree. Some number of Gauss-Seidel iterations are performed on all equations up to degree $p_{\max}$ where $p_{\max}$ is the maximum degree. Then the Gauss-Seidel iterations are applied to all equations up to degree $p_{\max} - 1$, then $p_{\max} - 2$, etc., until only the linear and quadratic equations are used. With the p-hierarchical basis, the "intergrid transfers" are automatic. Then the "coarse grid" equations (equations corresponding to the vertices, i.e. linear elements) are solved "exactly" by using a standard h-multigrid method. In PHAML, the h-hierarchical basis multigrid method is used, as follows. The residual is injected into the equations corresponding to the linear basis functions. The equations corresponding to the linear basis functions are relaxed by some red-black Gauss-Seidel iterations. The black equations are those corresponding to equations in the coarse grid, and the red equations are from the fine grid but not the coarse grid. A half iteration is allowed, which means relaxing the red equations but not the black. A basis change is then performed on those equations to convert from a nodal basis to a 2-level h-hierarchical basis, and the coarse grid equations are extracted. The process of relaxation, basis change and extraction is repeated until the grid consists only of the initial grid, i.e. all elements have refinement level 1. The coarsest grid problem is solved with a LAPACK direct solver. The process is then reversed by performing relaxation followed by conversion from 2-level h-hierarchical basis to nodal basis to get the next finer grid. After the finest level is reached, the second half of the p-multigrid cycle performs relaxations on all equations up to degree 2, then up to degree 3, etc. This constitutes one multigrid V-cycle. Cycles are repeated until some termination criterion is met. Finally, the equations corresponding to face basis functions are solved directly.

There are several arguments to `phaml_solve_pde` that determine the specifics of the multigrid algorithm. `mg_prerelax_ho` and `mg_postrelax_ho` determine the number of Gauss-Seidel iterations to perform on each level of the p-multigrid cycle, before and after solving the linear basis equations. `mg_prerelax` and `mg_postrelax` give the number of half-red-black Gauss-Seidel iterations to perform before and after solving the coarse grid problem for the linear equations. A half iteration relaxes the red equations but not the black equations. So, for example, `mg_prerelax=2` specifies one red-black iteration.

The termination of the multigrid cycles can be specified as a fixed number of cycles or by a tolerance on the residual of the linear system. To terminate by a tolerance, specify the tolerance in `mg_tol`. Iterations continue until the ℓ^2 norm of the residual of the scaled linear system is less than `mg_tol`. There are two symbolic constants that provide special values for `mg_tol`. `MG_ERREST_TOL` says to cycle until the residual is reduced to some fraction of the global error estimate. This avoids excess computation from solving the system more accurately than is necessary relative to the discretization error. `MG_NO_TOL` says to use a fixed number of iterations rather than a tolerance. The argument `mg_cycles` gives the fixed number of cycles to perform. Used in conjunction with a tolerance, `mg_cycles` provides an upper bound on the number of cycles to guarantee the iteration will terminate.

The HBMG as implemented in PHAML uses the full domain partition approach to parallelism by default [32]. This approach allows the use of only two messages in each h-multigrid cycle, one at the coarsest grid and one at the finest grid, with a (usually very minor) reduction in the convergence rate of the h-hierarchical basis multigrid method, but still uses communication after each level of the p-multigrid cycle. PHAML also provides the option of using conventional parallelism with messages on each h-level, which gives exactly the same results as the sequential HBMG. This is selected by specifying `mg_comm = MGCOMM_CONVENTIONAL`.

3.3.4.2 Krylov space solvers

PHAML also contains two Krylov space solvers: conjugate gradients and GMRES. For a description of these methods, see [9]. The methods are selected by setting `solver` to be `CG_SOLVER` and `GMRES_SOLVER`, respectively. As with the HBMG method, PHAML begins by eliminating the equations associated with face basis function by static condensation. It also eliminates the equations associated with Dirichlet boundary conditions so that the working matrix is symmetric.

Either method can be used without preconditioning via `preconditioner=NO_PRECONDITION` or with HBMG as the preconditioner via `preconditioner=MG_PRECONDITION`. As a preconditioner, HBMG does not need to converge to the solution, just give an approximation. It is usually sufficient to use two iterations, so the default HBMG parameters are set appropriately when HBMG is used as a preconditioner instead of a solver. Also, the HBMG preconditioner uses, by default, `ignore_quad_err=.true.` to avoid reducing the larger quadrature errors in unowned elements, and `mg_comm = MGCOMM_NONE` to skip the communication steps in HBMG.

There are three parameters that control the Krylov space solvers. `krylov_iter` provides an upper bound on the number of iterations allowed, and `krylov_tol` gives a tolerance on the ℓ^2 norm of the residual. Convergence is declared when the residual is less than the tolerance. If the maximum number of iterations is achieved before convergence, the solution is accepted and a warning is printed. `krylov_restart` gives the number of restart vectors for GMRES.

3.3.4.3 Alternative direct solvers

3.3.4.3.1 LAPACK

The LAPACK library [5] is always linked with a PHAML program. In limited situations it can be used as the linear system solver. It is specified by `solver=LAPACK_SPD_SOLVER` for most problems, which generate a symmetric positive definite matrix, or by `solver=LAPACK_INDEFINITE_SOLVER` for problems that generate an indefinite symmetric matrix. However, it can only be used as the solver for sequential programs because it is not a parallel library. And it should only be used for relatively small problems.

3.3.4.3.2 MUMPS

MUMPS [3][4] is a parallel direct solver from the European project PARASOL. It is accessed through PETSc, so PETSc must also be installed and be configured for MUMPS support. MUMPS is specified with `solver=PETSC_MUMPS_SPD_SOLVER` for the symmetric positive definite solver, or `solver=PETSC_MUMPS_GEN_SOLVER` for the nonsymmetric solver.

`PETSC_RICHARDSON_SOLVER`	Richardson
`PETSC_CHEBYCHEV_SOLVER`	Chebychev
`PETSC_CG_SOLVER`	conjugate gradients
`PETSC_BICG_SOLVER`	BiConjugate Gradients
`PETSC_GMRES_SOLVER`	generalized minimal residual
`PETSC_BCGS_SOLVER`	biconjugate gradients stabilized
`PETSC_CGS_SOLVER`	conjugate gradient squared
`PETSC_TCQMR_SOLVER`	transpose-free quasi-minimal residual
`PETSC_TFQMR_SOLVER`	transpose-free quasi-minimal residual
`PETSC_CR_SOLVER`	conjugate residual
`PETSC_LSQR_SOLVER`	least squares

Table 3.4: Available values of `solver` for the PETSc solvers.

`NO_PRECONDITION`	no preconditioning
`MG_PRECONDITION`	one hierarchical basis multigrid V-cycle
`PETSC_JACOBI_PRECONDITION`	Jacobi
`PETSC_BJACOBI_PRECONDITION`	block Jacobi
`PETSC_SOR_PRECONDITION`	SOR and SSOR
`PETSC_EISENSTAT_PRECONDITION`	SOR with Eisenstat trick
`PETSC_ICC_PRECONDITION`	incomplete Cholesky
`PETSC_ILU_PRECONDITION`	incomplete LU
`PETSC_ASM_PRECONDITION`	additive Schwarz
`PETSC_GAMG_PRECONDITION`	algebraic multigrid
`PETSC_TRILINOS_ML_PRECONDITION`	algebraic multigrid package ML from Trilinos

Table 3.5: Available values of `precondition` for the PETSc solvers.

3.3.4.3.3 SuperLU

SuperLU [26] is a parallel direct solver from the Lawrence Berkley National Laboratories. It is accessed through PETSc, so PETSc must also be installed and be configured for SuperLU support. SuperLU is specified with `solver=PETSC_SUPERLU_SOLVER`.

3.3.4.4 Alternative iterative solvers

3.3.4.4.1 PETSc

PETSc [7][8] is a parallel library of preconditioners and Krylov space iterative solvers from Argonne National Laboratories. PHAML provides access to most of the methods in PETSc and several parameters to those methods. Table 3.4 contains the available PETSc solvers as specified by `solver`. Table 3.5 contains the available preconditioners for the PETSc solvers specified by `preconditioner`.

There are a number of arguments that are used as parameters to the PETSc methods. These are listed in Table 3.6. Refer to the PETSc User's Manual [8]

real(my_real)	petsc_richardson_damping_factor
real(my_real)	petsc_chebychev_emin
real(my_real)	petsc_chebychev_emax
integer	petsc_gmres_max_steps
real(my_real)	petsc_rtol
real(my_real)	petsc_atol
real(my_real)	petsc_dtol
integer	petsc_maxits
integer	petsc_ilu_levels
integer	petsc_icc_levels
real(my_real)	petsc_ilu_dt
real(my_real)	petsc_ilu_dtcol
integer	petsc_ilu_maxrowcount
real(my_real)	petsc_sor_omega
integer	petsc_sor_its
integer	petsc_sor_lits
logical	petsc_eisenstat_nodiagscaling
real(my_real)	petsc_eisenstat_omega
integer	petsc_asm_overlap

Table 3.6: Arguments that are passed to the PETSc solvers.

for explanations of these arguments.

If the preconditioner is not one of the ones starting with `PETSC`, then memory can be saved by not copying the matrix to the PETSc format. This is specified by `petsc_matrix_free=.true.`

If you use PETSc, you might have to make some changes to PHAML depending on what version of PETSc you have. See `mkmkfile.sh`, `petsc_init.F90`, and `petsc_interf.F90` and search for "before" to see if you need to make changes.

3.3.4.4.2 *hypre*

hypre [16][17] is a package of parallel iterative solvers and preconditioners from Lawrence Livermore National Laboratories. It is accessed through PETSc, so PETSc must also be installed and be configured for *hypre* support. The four preconditioners from *hypre* that are available through PETSc are BoomerAMG, ParaSails, and Pilut. The are used in conjunction with a PETSc solver from Table 3.4. They are selected with `preconditioner = PETSC_HYPRE_xxx_PRECONDITION`, with `xxx` being `BOOMERAMG, PARASAILS` or `PILUT`. BoomerAMG can also be used as a solver via `solver = PETSC_HYPRE_BOOMERAMG_SOLVER`. There are several arguments that are passed to the *hypre* methods listed in Table 3.7. See the *hypre* reference manual (available at the *hypre* web site) for an explanation of these.

real(my_real)	hypre_BoomerAMG_tol
real(my_real)	hypre_BoomerAMG_trunc_factor
real(my_real)	hypre_BoomerAMG_strong_threshold
real(my_real)	hypre_BoomerAMG_max_row_sum
real(my_real)	hypre_BoomerAMG_relax_weight
real(my_real)	hypre_BoomerAMG_outer_relax_weight
integer	hypre_BoomerAMG_cycle_type
integer	hypre_BoomerAMG_max_levels
integer	hypre_BoomerAMG_max_iter
integer	hypre_BoomerAMG_P_max_elmts
integer	hypre_BoomerAMG_agg_num_levels
integer	hypre_BoomerAMG_agg_num_paths
integer	hypre_BoomerAMG_num_sweeps_all
integer	hypre_BoomerAMG_num_sweeps_down
integer	hypre_BoomerAMG_num_sweeps_up
integer	hypre_BoomerAMG_num_sweeps_coarsest
integer	hypre_BoomerAMG_relax_type_all
integer	hypre_BoomerAMG_relax_type_down
integer	hypre_BoomerAMG_relax_type_up
integer	hypre_BoomerAMG_relax_type_coarsest
integer	hypre_BoomerAMG_relax_order
integer	hypre_BoomerAMG_measure_type
integer	hypre_BoomerAMG_coarsen_type
integer	hypre_BoomerAMG_interp_type
logical	hypre_BoomerAMG_print_statistics
logical	hypre_BoomerAMG_print_debug
real(my_real)	hypre_Pilut_tol
integer	hypre_Pilut_maxiter
integer	hypre_Pilut_factorrowsize
real(my_real)	hypre_ParaSails_thresh
real(my_real)	hypre_ParaSails_filter
real(my_real)	hypre_ParaSails_loadbal
integer	hypre_ParaSails_nlevels
integer	hypre_ParaSails_sym
logical	hypre_ParaSails_logging
logical	hypre_ParaSails_reuse

Table 3.7: Arguments that are passed to the *hypre* solvers and preconditioners.

3.3.5 Load balancing

A parallel program with adaptive grid refinement must perform dynamic load balancing. When the grid is refined adaptively, some processors will perform more refinement than others, resulting in more grid elements, and hence more of the computational load, than others. Dynamic load balancing redistributes ownership of the elements to balance the load among the processors.

In PHAML, load balancing is performed by partitioning the grid into P sets where P is the number of slave processes. Each process is said to own the triangles in one of the partitions. Each vertex and edge has an associated triangle and is owned by the process that owns that triangle. PHAML uses a full domain partition (FuDoP) [31] in which each process also has additional coarse elements that cover the unowned part of the domain. Figure 3.5 illustrates an adaptively refined grid and the grid that would be seen by each of three processors, with the color indicating ownership.

One normally thinks of performing load balancing after refinement to redistribute the new grid. But it is also possible to perform predictive load balancing before refinement, which can reduce the amount of data to be redistributed. There also may be advantages to basing the balance on the number of elements, number of vertices or number of equations. PHAML provides the choice of balancing any of these entities before and/or after refinement. The number of entities (elements, vertices or equations) that are associated with an element is used as the weight for the element in the partitioning algorithms. For balancing after refinement, it divides up the number of entities as equally as possible. For balancing before refinement, it estimates the number of entities that will be associated after refinement. If `refterm` is not `ONE_REF` or `ONE_REF_HALF_ERRIND`, it includes the error indicator in the weight, so that those that are likely to be refined more times are given more weight. The selection of what to balance and when to balance is given by the arguments `prebalance` and `postbalance` which can take the value `BALANCE_NONE`, `BALANCE_ELEMENTS`, `BALANCE_VERTICES` or `BALANCE_EQUATIONS`. Usually, one of the two arguments is `BALANCE_NONE` so that either regular or predictive balancing is performed, but it is possible to perform balancing on both sides of refinement.

Grid partitioning algorithms have been the topic of extensive research, and there are several algorithms available. The method built into PHAML is the k-way refinement tree method [33]. This method uses the inherent refinement tree where the tree nodes correspond to triangles and the children of a tree node are the triangles created when a triangle is refined. Weights are attached to the leaf nodes and a tree traversal is performed to sum the weights. A second traversal is performed to partition the tree into P subtrees of equal summed weight. The children in the tree are ordered such that a tree traversal gives a space filling curve through the grid, and partitions are connected.

The choice of partitioning method is determined by the argument `partition_method`. The built in k-way refinement tree method is selected by the value `RTK`. Alternative partitioning methods are provided through the optional Zoltan dynamic load balancing library [14][15]. The values for selecting methods from Zoltan

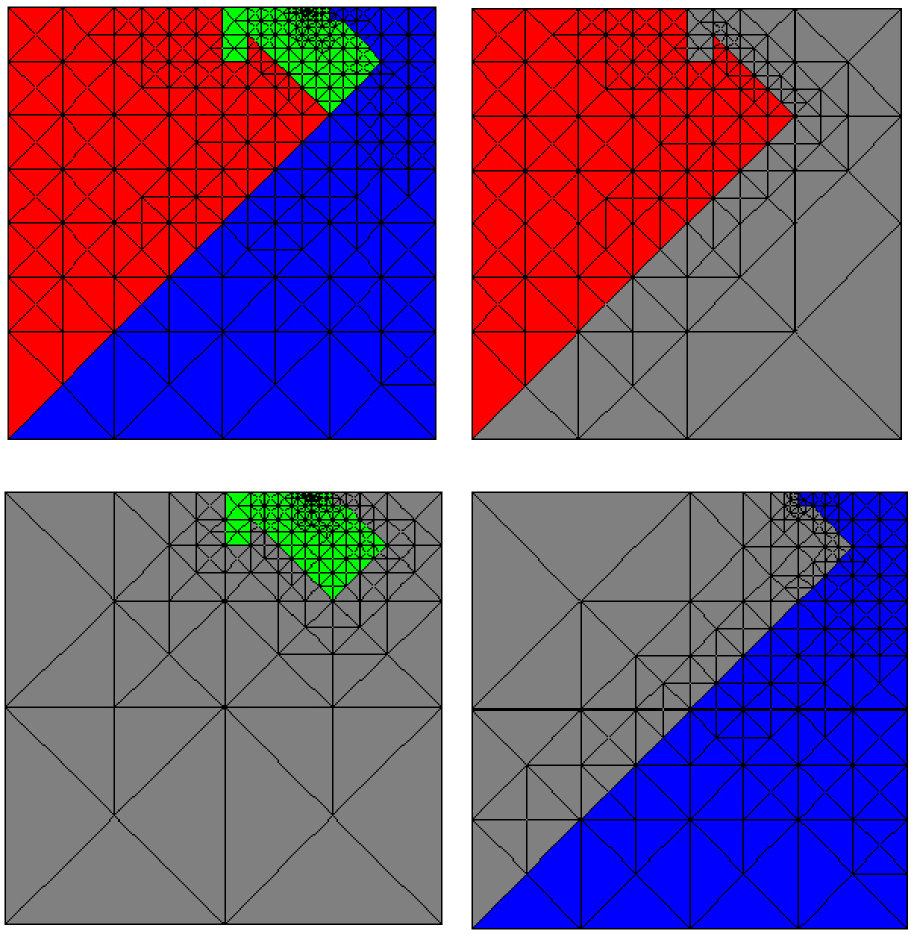


Figure 3.5: An adaptive grid partitioned for 3 processors, and the grid seen by each of the processors.

`ZOLTAN_RCB`	recursive coordinate bisection
`ZOLTAN_OCT`	RPI's Octree method
`ZOLTAN_METIS`	local diffusion method from ParMETIS
`ZOLTAN_REFTREE`	refinement tree
`ZOLTAN_RIB`	recursive inertial bisection
`ZOLTAN_HSFC`	Hilbert space filling curve
`ZOLTAN_FILE`	read Zoltan method and parameters from a file

Table 3.8: Available values of `partition_method` for Zoltan partitioners.

are given in Table 3.8. See the Zoltan User's Guide for descriptions of these methods, except ZOLTAN_FILE.

ZOLTAN_FILE lets you specify the method to use in Zoltan, and also to specify other Zoltan parameters, in a file. Basically, any parameter than can be set with Zoltan_Set_Param (see the Zoltan User's Guide) can be set by including a line containing the parameter name and value. In particular, you can specify the method with, for example, LB_METHOD RCB. For a full description of this file, see the zoltanParams web page [49]. The Zoltan parameter file is specified by the phaml_solve_pde argument zoltan_param_file, with a default value of "zoltan.params".

DRUM (the Dynamic Resource Utilization Model) [18][48] supports resource-aware, large-scale scientific computing in heterogeneous and hierarchical parallel computing environments. It can improve the load balance on, for example, clusters containing different kinds of processors. Within PHAML, DRUM is accessed with the partitioning method ZOLTAN_FILE. The parameters for DRUM are specified in the Zoltan parameter file. See the DRUM documentation for a description of the DRUM parameters.

3.3.6 Termination

There are several ways to specify how long phaml_solve_pde should continue to work on the solution, i.e. when to terminate. This section presents them. At least one of them must be specified or else the subroutine will run forever. Multiple termination criteria can be specified, and the routine will return when any of them are satisfied.

The argument task selects what task should be performed by phaml_solve_pde. Three of the values for task invoke a single pass of one part of the program, and no further termination criterion is needed. These are BALANCE_ONLY, REFINE_ONLY, and SOLVE_ONLY. The value BALANCE_REFINE_SOLVE invokes a loop over the three phases until one of the termination criteria is met. SET_INITIAL also loops over the three phases, but for the solve phase it interpolates the function in subroutine iconds (see Section 6.3.5). This is usually used for setting initial conditions for a time dependent problem, or an initial guess for a nonlinear problem (see Section 4.3).

The termination criteria are given by optional arguments and fall into two categories. The first is those that specify an upper bound on the number of something. These arguments all take an integer value. The arguments are max_elem (elements), max_vert (vertices), max_eq (equations in the linear system), and max_refsolveloop (number of times through the refine/solve loop). You can also specify max_lev (refinement levels) and max_deg (polynomial degree), but by default these are not termination criteria – if the refinement of an element would exceed the given value, then it is simply not performed. To use these as termination criteria, use the logical arguments stop_on_maxlev and stop_on_maxdeg.

The other category is to terminate when an error estimate is small enough. The global error estimate is computed from the local error indicator. The estimate can be an estimate of the energy norm, H^1 norm, H^1 semi-norm, L^∞ norm, or L^2 norm of the error. The arguments `term_energy_err`, `term_H1_err`, `term_H1_seminorm_err`, `term_Linf_err`, and `term_L2_err` all take a `real(my_real)` value. `term_H1_err` and `term_H1_seminorm_err` cannot be used in conjunction with the HIERARCHICAL_COEFFICIENT and EXPLICIT_ERRIND error estimators.

3.4 I/O

3.4.1 I/O files

PHAML writes printed output to two units, which can be specified through the integer arguments `output_unit` and `error_unit` of subroutine `phaml_create`. Error messages and warnings are written to `error_unit` and all other printed output is written to `output_unit`. By default, `output_unit` is 6 which most compilers provide as a pre-connected unit, often referred to as stdout. Also by default, `error_unit` is 0 which most compilers provide as a pre-connected unit, often referred to as stderr. If your compiler uses different unit numbers for pre-connected units, the correct units can be specified through these arguments. The two units can be the same if you want to have error messages and printed output intermixed. Warning messages from the master and slave processes can be suppressed by passing `print_warnings=.false.` to subroutine `phaml_solve_pde`. Error messages and warnings from graphics processes cannot be suppressed.

Usually stdout and stderr print to the terminal screen. In particular, they usually print to the window from which the program was started. However, the processes of a parallel program might not have an associated window, and the destination of stdout and stderr is determined by the parallel library. For example, if using a master/slave model with LAM as the parallel library, output from the master process will go to the window from which it was started, but output from the slave processes will go to the window from which `lamboot` was run. Moreover, output from all the slaves is intermixed in this window. To get more control over the destination of output from the slaves you can use `spawn_form=DEBUG_SLAVE` in `phaml_create`. This will open a window for each slave process and normally the printed output goes to those windows.

If you prefer to have the printed output directed to a file, then you can open a unit and specify that unit in `output_unit` and/or `error_unit`. PHAML provides "parallel open" and "parallel close" subroutines for this purpose. Subroutine `phaml_popen` (Section 6.4.11) opens a unit with a different file for the master and each of the slaves. If you specify the name of the file to be `root.suffix` then the actual filenames are `rootXXXX.suffix` for slave number XXXX, where the number of digits in XXXX is the minimum needed for the number of slaves. The master process is number 0. Subroutine `phaml_pclose` (Section 6.4.10) closes the unit.

Thus the usual process for directing printed output (or error) to files is: 1) call phaml_create with some non-pre-connected unit number in output_unit, 2) call phaml_popen with that unit number and some root file name, 3) call phaml_solve_pde, 4) call phaml_pclose with that unit number. Note that if there are any error messages printed by phaml_create, they cannot be written to this file because the unit has not yet been opened. These messages are written to unit 0 by default. You can specify a different unit through the argument output_now, but it must be a pre-connected unit.

3.4.2 Printed I/O

PHAML provides for the printing of various quantities at various times during the execution of phaml_solve_pde. By default, the only printed output is a header containing a summary of the input variables to phaml_solve_pde and a trailer containing termination information, printed by the master process. Other output is controlled through a series of "when" and "who" arguments. The "when" arguments indicate how often to print something. They take the values NEVER (don't print that quantity), FINAL (print it just before returning), PHASES (print it once in each refine/solve loop), and FREQUENTLY (print more often, usually used for debugging). The "who" arguments indicate which processes should print something. They take the values NO_ONE (don't print that quantity), MASTER (the master prints that quantity for the entire grid), SLAVES (each slave prints that quantity for the part of the grid that it owns), EVERYONE (both the master and the slaves print), and MASTER_ALL (the master prints the quantity for each of the slaves).

print_grid_when and print_grid_who provide for printing a summary of the grid, such as the number of vertices, number of elements, etc. print_linsys_when and print_linsys_who provide for printing a summary of the linear system, such as the number of equations, etc. print_solver_when and print_solver_who provide for printing a summary of the solver, such as the number of iterations used, the norm of the residual, etc.

print_error_when and print_error_who provide for printing certain norms of the error (if the true solution is provided) and error estimates. The logical arguments print_energy_norm_error, print_H1_norm_error, print_H1_seminorm_error, print_Linf_norm_error and print_L2_norm_error indicate whether or not to print the energy norm, H^1 norm, H^1 semi-norm, L^∞ norm and L^2 norm of the error, respectively. The default is .false. for all of them. The energy, H^1, H^1 semi-norm and L^2 errors are approximated using a sixth order quadrature rule for the integrals. The L^∞ norm is approximated using the quadrature points of a sixth order quadrature rule.

Similar arguments, but with "error" replaced by "errest" (e.g. print_energy_norm_errest), control whether or not the error estimates are printed.

The norms of the error and error estimates can be either absolute error (the default) or relative error. This is controlled by errtype which takes the values ABSOLUTE_ERROR and RELATIVE_ERROR. If the relative error is selected, then the printed norm of the error is divided by the norm of the true solution, and the printed error estimate is divided by the norm of the computed solution.

`print_error_when` also provides for monitoring the convergence rate of the iterative linear system solver, if the solver is the built-in hierarchical basis multigrid, conjugate gradients, or GMRES method or one of the solvers from PETSc. If it has the value `FREQUENTLY` then the ℓ^2 norm of the residual is printed after each iteration. For GMRES, it is printed at the restarts. It also accepts the value `TOO_MUCH` which additionally sets the solution to 0.0 before starting the iterations, to avoid convergence in 1 iteration.

`print_time_when` and `print_time_who` provide for measuring execution time of the program. The execution time of each section of the program (refinement, reconciliation, load balancing, matrix assembly, linear system solution, communication) is printed. Each time the time is printed it prints the time for the most recent pass through the refine/solve loop and the total time so far. `clocks` determines how the time is measured. It can be `CLOCK_C` for the cpu clock, `CLOCK_W` for the wall clock, or `CLOCK_CW` for both.

`print_header_who` and `print_trailer_who` specify which processes should print the header and trailer, respectively.

3.4.3 Pausing

In order to examine printed or graphical output while a PHAML program is running, it is often useful to have the program pause until you indicate that it may continue. There are several "pause" arguments to `phaml_solve_pde` that provide for this. They are `logical` arguments. When the program pauses, the master prints "`press return to continue`" to its printed output unit. It then reads from standard input, which is usually associated with the window from which the master program was run. The pause arguments are `pause_at_start` (pause upon entering `phaml_solve_pde`), `pause_at_end` (pause before leaving `phaml_solve_pde`), `pause_after_phases` (pause at the end of each refine/solve loop), and `pause_after_draw` (pause each time the graphics is updated).

3.5 Graphics

3.5.1 Overview

Graphics, or visualization, in PHAML is provided using OpenGL, which is a platform-independent specification of a graphics application programming interface, and GLUT, which supplies window, keyboard and mouse usage for OpenGL. There are libraries for both of these specifications available for nearly every computer. See Section 2.1.5 for URLs for more information on OpenGL and GLUT and how to obtain the software.

PHAML's graphics are interactive and menu driven. There may be graphics windows associated with the master process and/or with each of the slave processes. The master's graphics shows the grid and solution as a whole entity, whereas the slaves each show the grid and solution as they know it. The selection of which processes will have graphics is made with the argument

view modifier	⇒
element edge color	⇒
element interior color	⇒
function	⇒
contour plots	⇒
preprocess function	⇒
subelement resolution	⇒
color scheme	⇒
toggle lights	⇒
element label	⇒
edge label	⇒
vertex label	⇒
associated element	⇒
eigenfunction to use	⇒
component to use	⇒
component scale	⇒
space filling curve	⇒
grid offset	⇒
axes	⇒
crop (debug window)	
toggle color key	
write postscript	⇒

Table 3.9: The main graphics menu.

`draw_grid_who` to `phaml_create`, which can have the value `MASTER`, `SLAVES`, `EVERYONE`, or `NO_ONE`. There is no option to have only a subset of the slaves do graphics.

The graphics servers, which are separate processes in the parallel program, receive messages from the associated master or slave whenever the grid or solution changes. For a program under a sequential compilation of PHAML, the messages are passed by writing files to `/tmp`. For a master/slave program, the graphics servers are spawned automatically during the execution of subroutine `phaml_create`. For an SPMD program, the graphics servers should be included in the number of processes launched (see Section 2.4). For a sequential program, you must start the graphics server, `phaml_graphics`, from the command line. If a sequential program terminates abnormally, you must terminate `phaml_graphics` by hand, and should check `/tmp` for leftover files `phaml_message` and `phaml_lock`, and remove them if they exist.

All interaction with the graphics is performed with the mouse and arrow keys. The left and middle mouse buttons and arrow keys can be assigned various operations to change the view, as discussed in Section 3.5.3. By default, the left button rotates, the middle button zooms and the arrow keys pan. The right button brings up a menu of actions you can take to modify the graphics. The main menu is shown in Table 3.9. Menu items with a right arrow (⇒) bring up submenus.

The next section will show some of the visualizations that are available. The subsequent sections will discuss how to manipulate the graphics through the submenus.

3.5.2 Example visualizations

The PHAML graphics server has many options in the graphics menu. Primarily the graphics options are for different displays of the grid properties, functions over the grid, and the partitioning of the grid over the slaves. The functions that can be displayed include not only the computed solution, but also the true solution and error (if the true solution is given), and error estimates. In this section we present some examples of PHAML's graphics capability with very brief descriptions. The subsequent sections will discuss how to use the submenus to create these and other graphical displays.

Figure 3.6 shows several of the different ways you can display a function. Parts (a)–(f) show surface plots of the solution, which comes from using the menu to select function to be solution. Part (a) shows the surface with the triangle interiors colored by the solution value using the rainbow color scheme where blue represents small values and red represents large values. In part (b) the same function is shown with the grid added to the surface, drawn in black. Part (c) displays the grid in black on the surface, but selects element interior color to be transparent. Part (d) is the same but with hidden lines removed, which is achieved by selecting element interior color to be white so that the triangle faces hide the grid lines behind them. Part (e) also has the grid on the surface and hidden lines removed, but with the grid lines colored by solution value. Part (f) is a surface plot using the striped color scheme and placing contour lines on the surface. Parts (g)–(l) show 2D displays of the solution obtained by selecting function to be no function and viewing from straight above. Part (g) uses the striped color scheme with contour lines drawn in the x-y plane. Part (h) shows the solution using the rainbow color scheme. Part (i) adds the grid to the previous image, and part (j) colors the triangle interiors transparent and the grid lines with the solution value. Part (k) is simply a contour plot with no grid lines and the triangle interiors transparent. Finally, part (l) adds the coloring of the triangle interiors by the solution value using the gray scale color scheme.

Figure 3.7 shows some additional visualizations of the grid. Part (a) simply shows the grid drawn in black. Part (b) shows the regions in which the grid is coarse or fine by coloring the interiors of the triangles by the triangle size, using blue for small triangles and red for large. In part (c) the triangle interiors are colored by the polynomial degree of the triangle, for visualizing the effect of p- and hp-adaptive refinement. And in part (d) we use function ⇒ levels to create a hierarchy of grids based on refinement level.

Figure 3.8 shows a few of the ways you can visualize how the grid has been partitioned for distribution over the slaves during the load balancing step. In

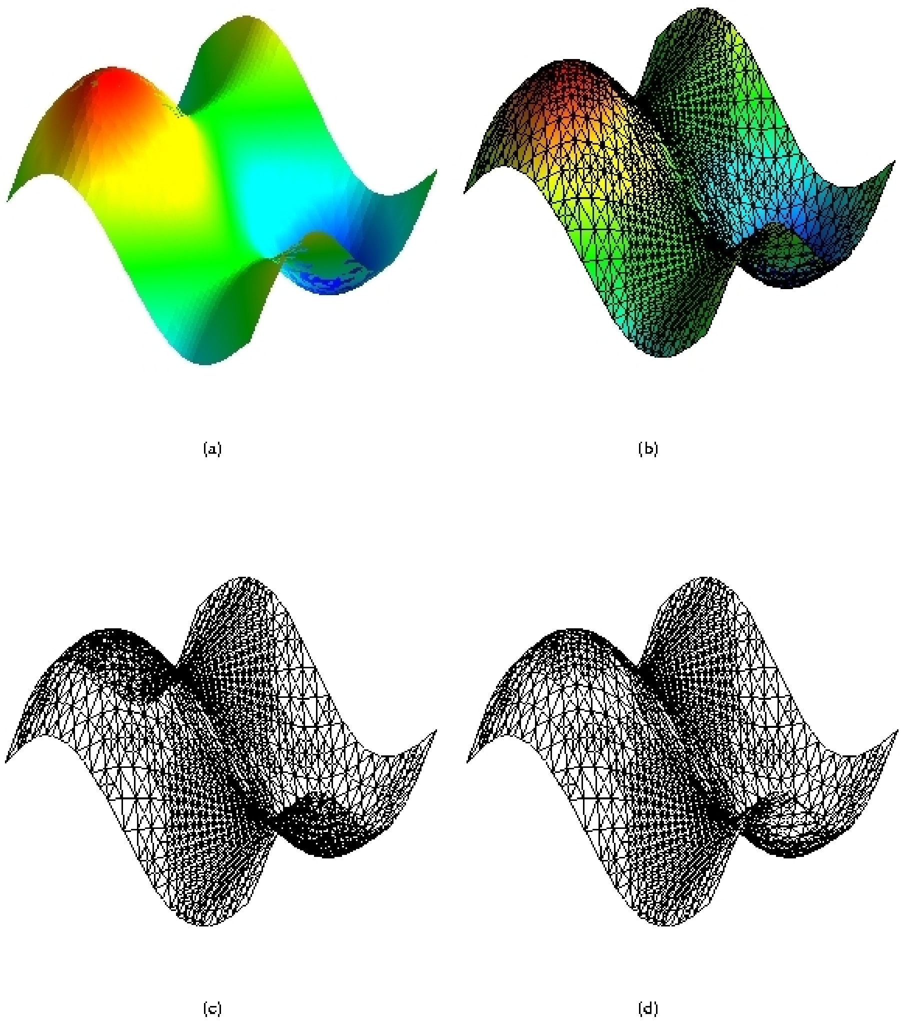
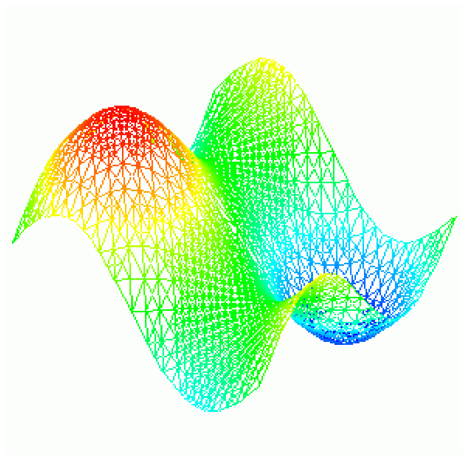
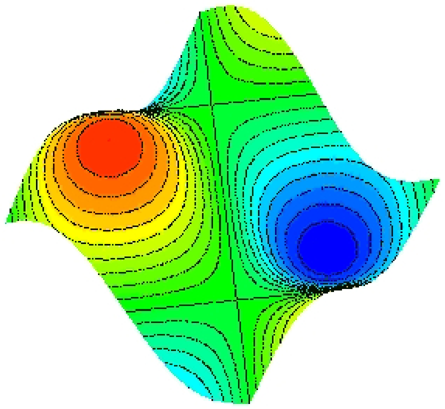


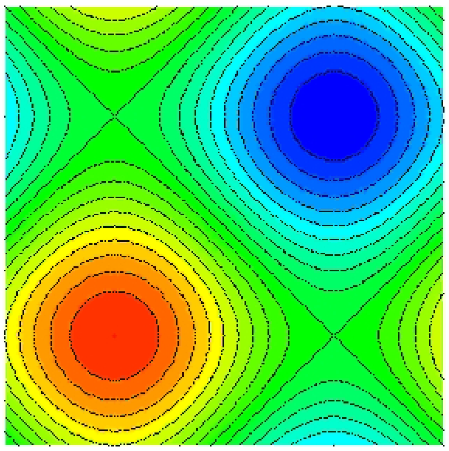
Figure 3.6: Visualizations of the solution.



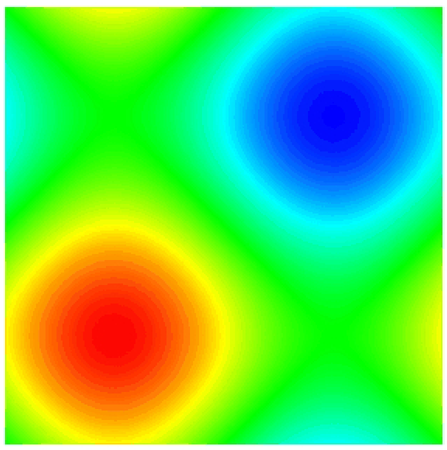
(e)



(f)

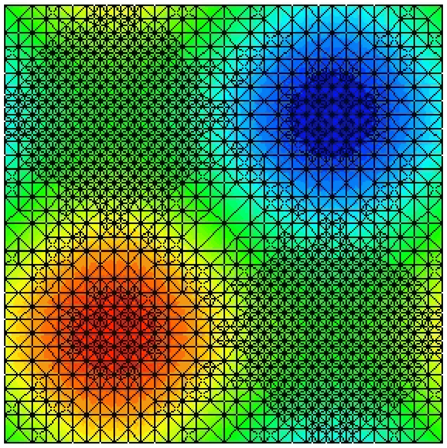


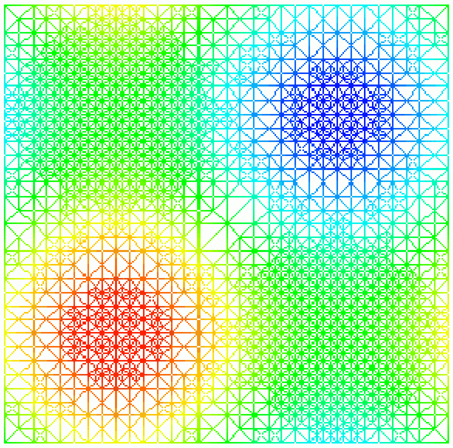
(g)

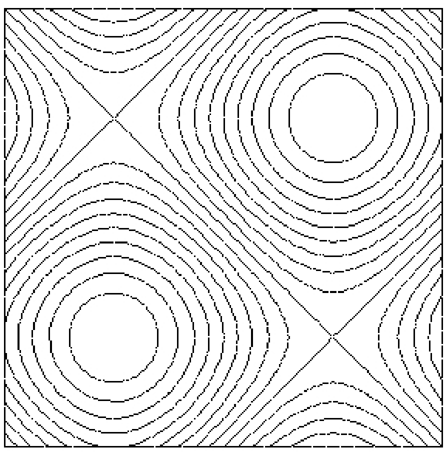


(h)

Figure 3.6: (continued) Visualizations of the solution.


(i)


(j)


(k)

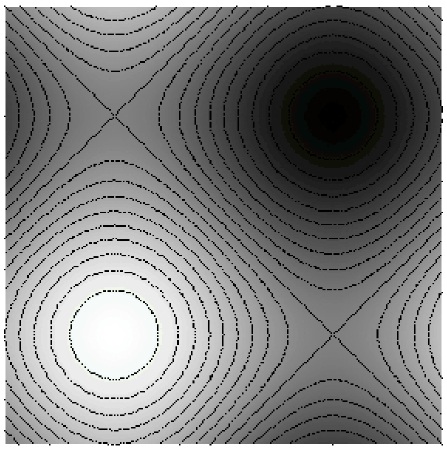

(l)

Figure 3.6: (continued) Visualizations of the solution.

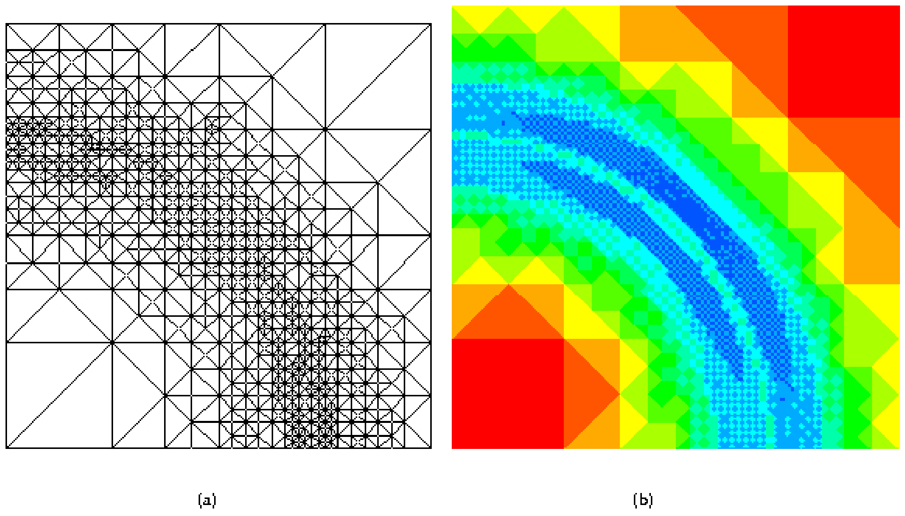
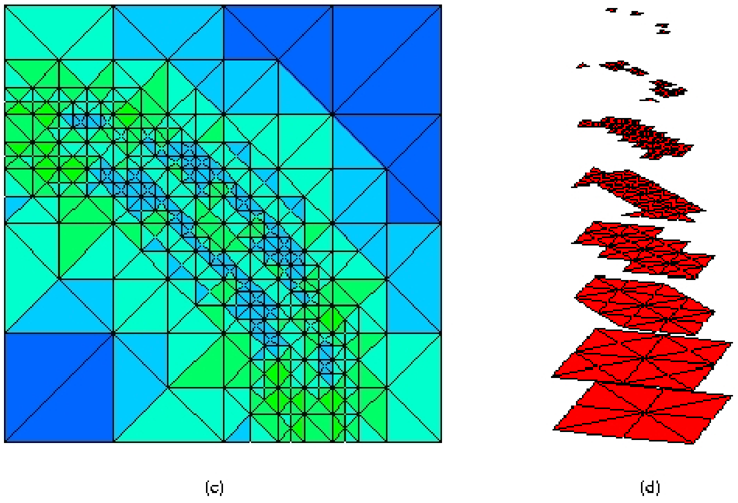



Figure 3.7: Visualizations of the grid.

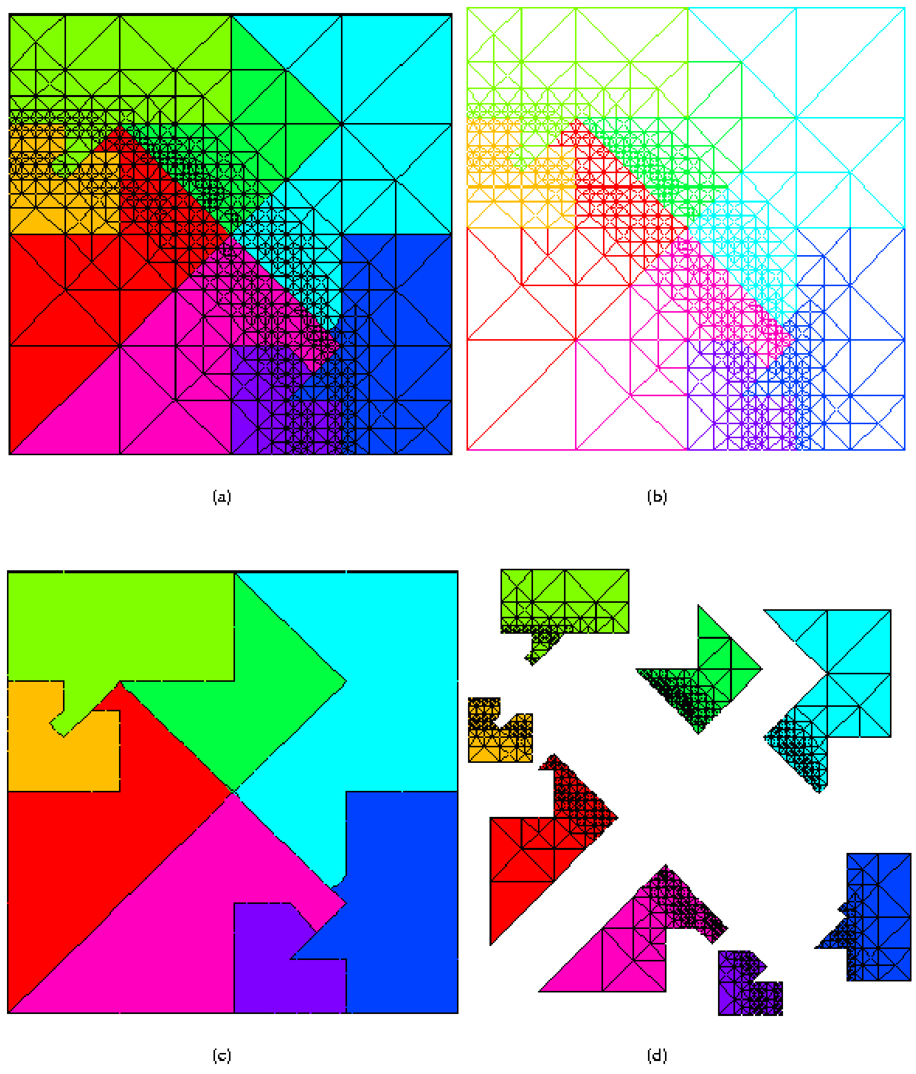


Figure 3.8: Visualizations of the partitions of the grid for load balancing.

left mouse button	⇒
middle mouse button	⇒
arrow keys	⇒
reset to initial view	
view from above	
view from above origin	
quit	

Table 3.10: The view modifier submenu.

part (a) the interior of the triangles is colored by owner and the grid lines are colored black. Part (b) colors the grid lines by owner and leaves the interior transparent. In part (c) the interiors are again colored by owner, but only the triangle edges that are on partition boundaries are drawn. Finally, part (d) shows an exploded grid where the partitions are physically separated.

3.5.3 View modifier

In this section, we discuss the view modifier. The view modifier submenu is shown in Table 3.10.

The first three items set the operation performed by the left mouse button, middle mouse button and arrow keys, respectively. The selected operation remains in effect until you select another one. The submenus below each of these are all the same. They contain rotate, zoom, pan, scale x (stretch or shrink along the x axis), scale y, scale z, explode (as in Figure 3.8(d)), and move light (see Section 3.5.6).

The next three entries are quick changes to a specific view of the grid. reset to initial view resets the rotation, zoom and pan settings to the original settings. view from above sets a view that looks straight down and at the center of the grid, with the (xmin,ymin) corner of the domain at the lower left corner of the image. This is normally used with function ⇒ no function for visualizations of the grid and contour plots. view from above origin looks at the point (0,0,0) from straight above. This is useful if you want to zoom in on the origin without having to pan repeatedly.

The final entry, quit, should not normally be used. If you terminate the graphics program using this menu item, it may or may not kill the master and/or slaves. The graphics program will terminate properly when `phaml_destroy` is called. Using the quit entry in the menu is only useful if the master or associated slave terminated early, and even then there might be a better way to terminate the graphics server (for example, with LAM the command `lamclean` will terminate all the processes).

no lines
black
edge owner
vertex owner
computed solution
true solution
error
size
degree
partition boundary black

Table 3.11: The element edge color submenu.

3.5.4 Colors

By default, PHAML uses a rainbow color scheme. Colorization of items that have a continuous numerical value, like the solution, comes from a continuous spectrum with blue corresponding to small values and red to large values. Normally the spectrum is scaled to correspond to the minimum and maximum values of the item begin drawn. Colorization of items that have a finite set of N discrete values, like the owner, comes from an equally spaced set of N colors in the spectrum from blue to red with blue assigned to the first item.

There are four other color schemes available. The color scheme is selected in the submenu under color scheme which has the selections rainbow, double rainbow, gray scale, striped, and stepped sequential. The double rainbow passes through the colors twice, with the second time a little more pastel. This is useful when discrete colors need more separation, such as when coloring by owner and there are a lot of processors, or when coloring by element degree with an *hp*-adaptive grid. The gray scale scheme uses a continuous gray scale from black to white with black corresponding to small values and white to large values. The striped scheme is like the rainbow scheme except the colors are from a discrete set of equally space colors from the spectrum from blue to red. The number of colors in the scheme is one less than the number of contour lines used for contour plots, so that contour lines will fall on the boundary between colors. The stepped sequential scheme uses several steps of saturation/value within each of several hues ranging from red to violet. The number of steps and number of hues can be changed by use of a submenu. By default, there are 4 steps of 6 hues for a total of 24 colors. This scheme is particularly useful for discrete values such as owner and degree.

With a color scheme selected, you can choose how to color the grid lines (i.e. element edges) and triangles (i.e. element interiors) to get different information about the grid, partition, solution, error, etc. Table 3.11 shows the element edge color submenu for selecting how to color the element edges. no lines means don't draw the grid. black draws the edges black for a simple drawing of the grid. edge owner selects the color to indicate which slave process owns each edge. vertex owner selects the color to indicate the owner of the vertices at the ends of each edge. If the owners of the two endpoints are different, the color blends from one to the other along the length of the edge. computed solution uses the color corresponding to the value of the computed solution at the endpoints, and blends the colors along the length of the edge. true solution is similar but uses the true solution if it is given in function `trues`. Likewise, error uses the computed solution minus the true solution, if it is available. size colors the edges according to their length, using red for the largest edges and blue for the smallest. This is useful for distinguishing element sizes when the grid is so fine that drawing the edges black would result in large black areas. degree colors the edges by the polynomial degree of the approximation space along that edge. Finally, partition boundary black draws only the edges that fall between two triangles with different owners, and edges on the domain boundary. This results in the partition boundary being drawn black.

The submenu for element interior color is similar to the one for element edge color, with just a few differences. The no lines entry is replaced by transparent, but has the same meaning of don't draw the element. black is replaced by white. Coloring an element interior white, which is the same as the graphics window background, has the effect of blocking whatever is behind the element, and can be used to draw hidden line plots. There is only one owner entry, used to indicate which slave owns each element. computed solution, true solution, error, size, and degree all have the same meaning as with edge color. There is no partition boundary entry. It has an additional entry for coloring each element by its error indicator.

3.5.5 Functions

The function submenu determines what function to draw as surface plots and contour plots. This menu has six entries. The first is no function, which simply draws the elements in the x-y plane. This is usually used in conjunction with viewing from above. The next three entries are computed solution, true solution, and error. They draw the corresponding function. The fifth entry is levels. This draws the elements, including parent elements, in L discrete planes parallel to the x-y plane, where L is the number of refinement levels in the grid (see Figure 3.7(d)). Each level contains the elements of that refinement level. You may find it useful to use scale z from the view modifier (Section 3.5.3) with this. The final entry is error indicator. This is a piecewise constant function with each element drawn at the height corresponding to its error indicator.

The functions (except levels) can be preprocessed in several ways with the submenu under preprocess function. The menu entries indicate what would be applied to a function f. They are none (no preprocessing, the default), -f (negate), abs(f) (absolute value), f**2 (square), and log(abs(f)) (logarithm of the absolute value).

3.5.6 Lights

When the function is no function, levels or an error estimate, or the striped color scheme is used, the image is rendered in flat light. Otherwise, it is rendered with a light source resulting in a 3D appearance with shadows. There are five lights available in the PHAML graphics. Four of them are fixed in position: one to the right, one to the left, one above and one below. The fifth light is movable. The default is that only the light to the right is turned on. Lights can be turned on and off with the submenu under toggle lights. The movable light can be moved with the mouse or arrow keys by selecting move light under the view modifier submenu.

3.5.7 Contour plots

In addition to being drawn as a surface or being represented by color, a function can be drawn as a contour plot. Contour plots are controlled by the submenu under contour plots. This submenu has four entries for selecting what function to plot, and three submenus for changing the properties of the contour plot.

The first four entries in the contour plot submenu select the function to plot. As usual, they are no contour plot, computed solution, true solution, and error. By default, no contour plot is drawn.

The next entry is set number of uniform lines. Initially PHAML uses 21 equally spaced contour values between the minimum and maximum values of the function. This submenu allows you to change the number of values while keeping them equally spaced. There are six entries that allow you to make the change directly from the menu: increment by 1, decrement by 1, increment by 10, decrement by 10, double, and cut in half. The final entry, enter number in debug window, lets you type in the number of contour lines you want. However, it prompts for this number from standard input, so the graphics process must have an associated window. This is achieved by using `spawn_form = DEBUG_GRAPHICS` or `spawn_form = DEBUG_BOTH` in the call to `phaml_create` (see Section 6.4.4).

You can also space the contour lines nonuniformly by using set nonuniform lines. This also requires a debug window. You will be prompted for the number of contour lines, and then to enter a comma separated list of the values for the contour lines.

The final menu entry gives two choices for the placement of the contours. They can either be placed on the x-y plane, or be elevated by the function value, i.e., placed on the surface.

3.5.8 Multiple solutions

If you solve a coupled system of equations (multicomponent solution) or solve for more than one eigenvalue of an eigenvalue problem, then there is more than one solution to draw. Two submenus let you select which function to display. The default is to display the first one.

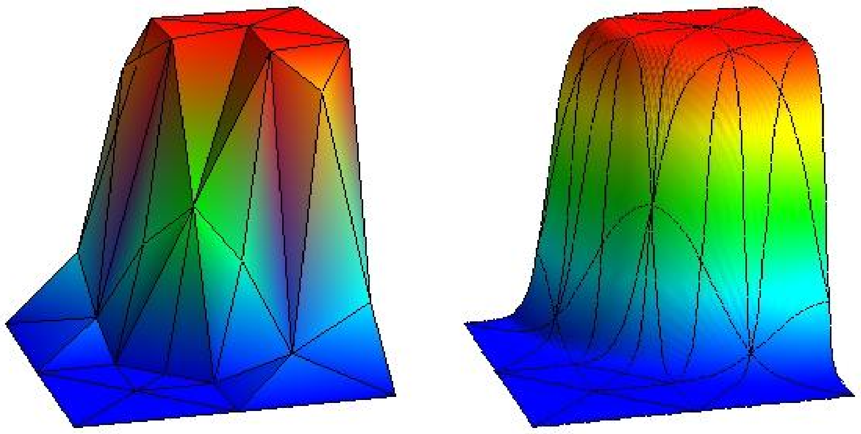


Figure 3.9: Improvement of a surface visualization by using subelement resolution.

eigenfunction to use provides the selection of which eigenfunction to display. It has an entry of the form eigenfunction 1, eigenfunction 2, etc., up to the number of eigenvalues computed. If there are more than 9 eigenvalues, the last entry is more $\Rightarrow$. This brings up a submenu containing 10's $\Rightarrow$, 20's $\Rightarrow$, etc. Under these submenus you will find the eigenfunctions with larger indices. PHAML sorts the eigenvalues from smallest to largest, and orders the corresponding eigenfunctions the same way.

component to use provides the selection of which component of a multi-component solution to display. It contains entries of the form component 1, component 2, etc. Like the eigenfunction selection, there are submenus for the higher indices if there are more than 9 components. The menu also contains two entries for displaying a composite of the components. If the components of the solution are u_1, u_2, $\ldots$, then L1 sum will display $|u_1| + |u_2| + \ldots$, and L2 sum will display $u_1^2 + u_2^2 + \ldots$

component scale provides the selection of how to scale the components when the function is computed solution, true solution or error. Normally the function is scaled by its maximum absolute value. For multicomponent solutions, you can choose to have each component scaled by its own maximum absolute value by selecting individual, or you can choose to have all components scaled the same using the maximum absolute value over all components by selecting all the same.

3.5.9 Miscellaneous features

This section addresses some menu items that are not big enough to warrant a section of their own.

The subelement resolution submenu is useful when high order elements are used. By default, a triangle is drawn as a piece of a plane defined by the three vertices of the triangle. Color blending, contour lines, etc., are also limited by this definition. This applies both to 3D surfaces and 2D drawings in the x-y plane. This is fine for piecewise linear elements since the solution is a plane over each triangle. But with higher order element, any detail on the subelement level is lost. This menu entry defines how much subelement resolution to use. The drawing is still done by drawing pieces of a plane, i.e. triangles, but multiple triangles are drawn within a grid element. With subelement level 0, the element is drawn as a single triangle (the default). With subelement level 1, the element is drawn as 4 triangles, formed by connecting the midpoints of the element edges. At subelement level 2, each of those 4 triangles are drawn as 4 triangles by connecting the midpoints of their sides, resulting in 16 triangles in a grid element. In general, subelement level ℓ results in drawing 4^ℓ triangles in each element. The effect of using a high level of subelement resolution can be seen in Figure 3.9.

subelement resolution has entries for 0, 1, 2 and 3 levels of subelement resolution. Since the number of triangles drawn grows exponentially with the number of subelement levels, using higher values of subelement resolution can be very slow. However, if needed, values larger than 3 are obtainable with the submenu entries increase, which adds 1, and decrease, which subtracts 1.

Axes can be added and removed from the plot with the axes submenu.

x, y and z axes can be added and removed from the plot by selecting standard axes and then toggle standard axes. The axes are fairly primitive with tic marks and values only at the ends and midpoint.

You can also define your own custom axes by selecting user defined axes. Submenu items are toggle defined axes, add axis, change axis, and remove axis. Use of this feature requires that the graphics process be run in a debug window, e.g. using `spawn_form=DEBUG_GRAPHICS` in `phaml_create`. When add, change or remove is selected, you will be prompted for input in the debug window. A new axis is defined by providing the (x, y, z) coordinates of the end points of the axis, and the number of tick marks for the axis.

A color key can be added and removed with the toggle color key entry. The key gives the correspondence between the color of the interior of the elements and numeric values. Figure 3.10 illustrates two uses of the color key: a continuous color key for the function value using the rainbow color scheme, and a discrete color key showing the element degree using the stepped sequential color scheme.

crop (debug window) provides a means of restricting how much of the domain is used in the display. Since it requires input from standard input, the graphics process must have an associated window. This is achieved by using `spawn_form = DEBUG_GRAPHICS` or `spawn_form = DEBUG_BOTH` in the call to `phaml_create` (see Section 6.4.4). When this menu entry is selected, it will prompt for the crop region to be entered as xmin, xmax, ymin, ymax.

The grid offset submenu helps to solve a potential problem with the rendering of the graphics. The elements are drawn as triangles and the grid lines are drawn as lines separately, but they occupy the same space. This can cause a problem

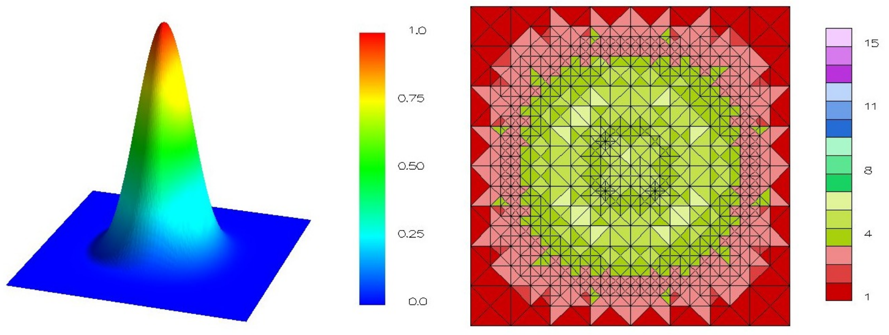


Figure 3.10: Examples of the color key.

in determining which should show when the image is rendered. Even if they are separated very slightly, there can be a problem because of machine roundoff error. This submenu allows you to change how far the grid lines are offset from the triangles. If you find that grid lines are disappearing, you should increase the offset. If you find that the grid lines appear to be separated from the surface, you should decrease the offset. The submenu entries let you increase or decrease by 1 or 10 at a time.

3.5.10 Development aids

Some of the graphics options were created as aids in the development and debugging of PHAML. These are probably not much use to the end user. They are the element label, edge label, and vertex label, which label each entity with its index in PHAML's data structure, associated element which displays the edge-element and vertex-element correspondence used to determine the owner of edges and vertices, and space filling curve which displays the space filling curve associated with the refinement tree partition method.

3.5.11 Postscript

The write postscript submenu lets you save the current visualization to an encapsulated postscript file. It writes vector graphics in the postscript language. This means the saved image is high quality and scalable, but it creates very large files. If you want smaller files you can use a screen capturing program and save the image in a raster graphics format like JPEG.

write postscript has two options in the submenu: unsorted and sorted. The sorting option sorts the entities of the image by distance from the viewer before writing the postscript file. There isn't really any reason to use the unsorted option, and it will probably be removed in the future.

When write postscript is selected, it creates a file called `renderX.eps` where X is 0 for the master's graphics processor or the slave number for the slaves' graphics processors (note there cannot be more than 9 slaves for this to work properly). The location of this file is compiler dependent, but it usually ends up in the directory where the master program was started or in the user's home directory. You may have to modify this file slightly in two ways. First, rename it to something more meaningful! Second, some printers need to have `showpage` added as the last command in the file, but that confuses some viewers. If you try to print the file and nothing happens, add this line.

3.6 Post-solution utilities

3.6.1 Store and Restore

There are times when it may be useful to save a PHAML solution and use it in some subsequent program. For example, one might solve a problem on a batch-only system and save the solution, and then later run a program on an interactive system that reads the solution and displays it with PHAML's graphics capability. PHAML provides a routine that writes the entire contents of a `phaml_solution_type` variable to a set of files (one file for the master and one for each slave), and a routine that reads those files into a `phaml_solution_type` variable. The files should be connected to a unit number using `phaml_popen` and `phaml_pclose` as described in section 3.4.1.

`phaml_store` takes two arguments: a `phaml_solution_type` variable and an integer specifying the unit to write to. `phaml_restore` also takes a `phaml_solution_type` variable (which should first be created with `phaml_create`, but otherwise be empty) and a unit to read from. It also takes two optional logical arguments. `do_draw_grid` indicates whether or not you want to invoke graphical output immediately after reading the file, and `pause` indicates whether or not to pause after the graphics. A program that reads files with `phaml_restore` must have the same number of slaves as the program that created the files with `phaml_store`.

3.6.2 Store Matrix

One might wish to store the linear system that represents the discretized PDE in a file for processing external to PHAML, for example solving the linear system with Matlab. Subroutine `phaml_store_matrix` does this. This routine stores the discretized PDE in phaml_solution so that it can be processed by an external program. In addition to a `phaml_solution_type` variable, it takes four optional arguments, `stiffness_unit`, `rhs_unit`, `mass_unit`, and `inc_quad_order`. `inc_quad_order` increases the order of the quadrature rule used for computing the matrix and right hand side entries, the same as in `phaml_solve_pde`.

For an elliptic boundary value problem, the discrete problem is a linear system of equations, $Ax = b$. `phaml_store_matrix` can store the stiffness matrix, A, and/or the right hand side, b. The presence of the optional arguments `stiffness_unit` and `rhs_unit` determines whether or not the stiffness matrix and right hand side will be stored, respectively. Either or both can be present.

`mass_unit` should not be present.

Two details about the stored matrix: First, the matrix is stored without static condensation. Second, the Dirichlet boundary conditions are pre-eliminated from the stored linear system, although the corresponding rows of the matrix are kept to maintain the same indexing of the unknowns. A row in the matrix corresponding to a Dirichlet point is replaced by an identity row, i.e. 1 on the diagonal and 0 elsewhere, and the corresponding right hand side is replaced with the Dirichlet value. To maintain symmetry, the corresponding column is replaced with an identity column and the right hand side is adjusted by subtracting the eliminated column entries times the Dirichlet values.

For an elliptic eigenvalue problem, the discrete problem is a generalized eigenvalue problem $Ax = \lambda Mx$. `phaml_store_matrix` can store the stiffness matrix, A, and/or the mass matrix, M. The presence of the optional arguments `stiffness_unit` and `mass_unit` determines whether or not the stiffness matrix and mass matrix will be stored, respectively. Either or both can be present. `rhs_unit` should not be present.

When present, `stiffness_unit`, `rhs_unit` and `mass_unit` should contain the I/O unit of a file. It is the responsibility of the calling program to open the unit for formatted, sequential writing before calling `phaml_store_matrix` and closing it after. This is done with the usual Fortran `open` and `close` statements, not the PHAML `phaml_popen` and `phaml_pclose` statements. If more than one is present, they must not be the same file.

The matrices are written in the Matrix Market exchange format. See `http://math.nist.gov/MatrixMarket/` for a description of the format and routines for reading the format in Fortran, C and Matlab. They are written in the real, general, coordinate format. The right hand side vector is written as an $N \times 1$ matrix in the real, general, coordinate Matrix Market format.

3.6.3 Store Grid

The grid, and optionally solution, can be stored to data files using `phaml_store_grid`. In 2D, the files can be stored in triangle's `.poly` format (see `http://www.cs.cmu.edu/~quake/triangle.poly.html`) by specifying `fmt=GRIDFILE_POLY` to store it without the solution, or `GRIDFILE_POLY_SOLN` to store it with the solution. The solution is stored as attributes of the vertices, so for high order solutions only the linear part is stored. The other triangle files (`.node`, `.neigh`, etc.) can be created from the `.poly` file using
`triangle -pneQY` *filename*`.poly`.
If the domain has holes, then the `boundary_` routines (Sect. 3.2.3) must be available, i.e., the initial grid cannot be specified by triangle files.

In 2D or 3D, the files can be stored in Gmsh's `.msh` format (see `http://geuz.org/gmsh/doc/texinfo/gmsh.html#MSH-ASCII-file-format`) by specifying `fmt=GRIDFILE_MSH` to store it without the solution, or `GRIDFILE_MSH_SOLN` to store it with the solution. The solution is stored as a NodeData section, so for high order solutions only the linear part is stored. If there are any tags attached to the grid entities, they are included in the .msh file unless `notags` is present and `.true.` The Elements section contains not only the grid elements (triangles in 2D and tetrahedra in 3D), but also the boundary vertices, boundary edges, and, in 3D, boundary faces unless `noboundary` or `only_gmsh` is present and `.true.` (`only_gmsh` only applies to 3D grids.) If `noboundary` is `.true.`, boundary entities are not included. If `noboundary` is `.false.` or not present, and `only_gmsh` is `.true.`, then vertices, edges and faces that were "elements" in the original geo or msh file, and their descendants, are included, but no other boundary entities. For boundary entities, the first tag is set to the boundary marker (Sects 3.2.2, 3.2.3). This tag is included even if `notags` is `.true.`

`comp` and `eigen` are optional arguments to control which components of a multicomponent solution and which eigenfunctions of an eigenvalue problem with multiple eigenvalues are stored. If `comp` is present, then it indicates which component to store. If it is not present, then all components are stored. If `eigen` is present, then it indicates with eigenfunction to store. If it is not present, then all eigenfunctions are stored. If neither `comp` nor `eigen` is present in a multicomponent, multieigenvalue problem with n components and m eigenvalues, then the order of the solution values in the data file is (comp 1, eigen 1), (comp 2, eigen 1), ..., (comp n, eigen 1), (comp 1, eigen 2), (comp 2, eigen 2), ... (comp n, eigen m).

In this release, storing the grid is restricted to one processor, i.e., PHAML must be built for sequential or OpenMP execution, or, if it is built for hybrid or MPI execution, you must specify `nproc=1`.

3.6.4 Query

PHAML provides for the recovery of many quantities of interest through subroutine `phaml_query`, which can be called after returning from `phaml_solve_pde`. This includes information about the grid, such as number of elements, number of vertices, minimum and maximum polynomial degree, etc. Most of them can be for the whole grid or for the grid that each slave has. A second category includes error estimates in various norms, and, if the true solution is provided, the norms of the error and true solution. The norms of the error are absolute error; you can get the relative error by dividing by the norm of the solution. A third category provides interesting quantities related to eigenvalue problems.

For a complete list of the quantities that can be recovered through `phaml_query`, see Section 6.4.12.

3.6.5 Solution evaluation

PHAML provides for evaluating the computed solution and its derivatives at a point in the domain through subroutine `phaml_evaluate` (see Section 6.4.6). After returning from `phaml_solve_pde`, you can pass the `phaml_solution_type` variable to `phaml_evaluate` to obtain the solution and/or first and second derivatives. You can request any subset of them. You also pass two arrays, `x` and `y`, containing the points at which to evaluate the solution. The solution is returned in the arrays `u`, `ux`, `uy`, `uxx` and `uyy`, which must have the same dimension as `x` and `y`. These are all optional arguments, and which ones are present determines which ones are evaluated. If you are solving a system of equations or an eigenvalue problems, there are optional arguments to specify which component or eigenfunction you want to evaluate. If a point outside the domain is given, the solution is returned as 0.

Another way to obtain the solution for post processing is through the subroutine `phaml_get_grid_soln` (see Section 6.4.7). This routine returns the vertices of the triangles in the grid in two arrays, `x` and `y`, and the solution at the vertices in the array `u`. The vertices are not returned in any particular order relative to their placement in the domain. If you are solving a system of equations or an eigenvalue problem, there are optional arguments to specify which component or eigenfunction you want to evaluate.

There is also a subroutine to evaluate an "old" solution, which can be used for time dependent and nonlinear problems. See Section 4.3 for information on this routine.

3.6.6 Functionals

In this context, a functional of the solution is some form of integral of the computed solution. Subroutine `phaml_integrate` (see Section 6.4.9) computes

$$\iint_{\Omega} k(x,y)\ u_i^p(x,y)\ u_j^q(x,y)\ dx\ dy.$$

u_i and u_j are two components of the solution of a system of equations, or two eigenfunctions of an eigenvalue problem, or u_i is a solution and u_j is 1. p and q are integer powers. k is a kernel function defined by the user in function `phaml_integral_kernel` (Section 6.3.7). In addition to a point at which to evaluate the kernel, the function takes an integer, `kernel`, which allows for the definition of several kernel functions in the same subroutine.

Chapter 4

Problem Extensions

4.1 Eigenvalue Problems

In addition to elliptic boundary value problems, PHAML can solve elliptic eigenvalue problems of the form

$$-\frac{\partial}{\partial x}\left(c_{xx}\frac{\partial u}{\partial x}\right)-\frac{\partial}{\partial x}\left(c_{xy}\frac{\partial u}{\partial y}\right)-\frac{\partial}{\partial y}\left(c_{yy}\frac{\partial u}{\partial y}\right)+c_x\frac{\partial u}{\partial x}+c_y\frac{\partial u}{\partial y}+c_u u = \lambda f u \text{ in } \Omega \tag{4.1}$$

$$u = 0 \text{ on } \partial\Omega_D \tag{4.2}$$

$$\left(c_{xx}\frac{\partial u}{\partial x}+c_{xy}\frac{\partial u}{\partial y}\right)\frac{\partial y}{\partial s}-c_{yy}\frac{\partial u}{\partial y}\frac{\partial x}{\partial s}+c_{bc}u = 0 \text{ on } \partial\Omega_N \tag{4.3}$$

Note that the boundary conditions must be homogeneous. Usually the function f is identically 1. However there are some occasions where other f are useful. For example, to put the Laplacian operator in polar coordinates into the form of Equation 4.1, one may multiply the canonical form of the equation by x (a.k.a. r in polar coordinates) which results in $f = x$.

You indicate that an eigenvalue problem is being solved by specifying `eq_type = EIGENVALUE` in subroutine `phaml_create`. The solution returns eigenfunctions, u, and the corresponding eigenvalues λ. More than one eigenpair can be computed. The number of desired eigenpairs is specified through the argument `num_eval` to subroutine `phaml_solve_pde`. Subroutines `phaml_evaluate`, `phaml_evaluate_old`, `phaml_integrate`, `phaml_query`, and `phaml_scale` take an optional integer argument, `eigen`, which specifies which eigenfunction to use. Subroutine `phaml_query` returns the entire set of eigenvalues in the `real(my_real)` array argument `eigenvalues`. Printed output prints all of the eigenpairs.

The discrete eigenvalue problem is solved using SLEPc or one of the external packages supported by SLEPc (ARPACK and BLOPEX). You should read the SLEPc User's Guide [11] to understand the arguments that effect the

SLEPc solvers. Not all methods are valid for all problems, and not all combinations of arguments are valid. The method to use for solving the eigenproblem is specified by `eigensolver`. Valid values are `SLEPC_POWER`, `SLEPC_SUBSPACE`, `SLEPC_ARNOLDI`, `SLEPC_LANCZOS`, `SLEPC_KRYLOV_SCHUR`, `SLEPC_GEN_DAVIDSON`, `SLEPC_JACOBI_DAVIDSON`, `SLEPC_LAPACK`, `SLEPC_ARPACK`, and `SLEPC_BLOPEX`.

By default PHAML computes the smallest eigenvalue(s). You can compute eigenvalues in the interior of the spectrum by using the argument `lambda0` to `phaml_solve_pde`. PHAML will compute the eigenvalues that are closest to `lambda0`. Convergence to an interior eigenvalue can be accelerated by using harmonic extraction, specified by `harmonic_extraction=.true.`, or by using a spectral transformation, specified by `transformation`. Valid values are `ST_NONE`, `ST_SHIFT_ORIGIN`, `ST_SHIFT_INVERT` and `ST_CAYLEY`. The transformations use a shift which, by default, is `lambda0`, but can be specified to be a different number using `st_shift`. The Cayley spectral transform also has an antishift which, by default, is the same as the shift, but can be specified with `st_antishift`.

Some solvers (e.g., Krylov solvers) can avoid computing the residual by using a cheap estimate of the residual norm, but this may sometimes give inaccurate results, especially if a spectral transform is being used. If this is a problem, you can force computation of the true residual with `slepc_true_residual=.true.`.

PHAML's default size of the subspace used by the solvers, a.k.a. number of column vectors, is the same as SLEPc's default. A different size can be specified with `eigen_ncv`. Termination of the eigensolver is controlled by two parameters, `eigen_tol` and `eigen_maxit`. `eigen_tol` is a tolerance for the error estimate of the eigenvalues and has a default value of 10^{-10}. `eigen_maxit` gives the maximum number of iterations allowed and has the same default value as SLEPc.

If u is a solution of Equation 4.1, then so is αu for any scalar number α. Thus the solution must be scaled to meet some condition to be unique. PHAML provides three options for how to scale the eigenfunctions through the argument `scale_evec` to subroutine `phaml_solve_pde`. `SCALE_LINF` requests that the ℓ^∞ norm of the eigenvector, x, of the discrete problem be 1. With linear elements, this is the same as the L^∞ norm of the eigenfunction u. `SCALE_L2` scales such that the ℓ^2 norm of x is 1. `SCALE_M` scales such that the M norm of the eigenvector, $\sqrt{x^T M x}$ where M is the mass matrix, or equivalently the L^2 norm of the eigenfunction, is 1.

The eigensolver requires the use of a linear system solver and sometimes a preconditioner. These are specified through `solver` and `preconditioner`. They must be solvers and preconditioners that are available through PETSc, including the `PETSC_MUMPS` and `PETSC_SUPERLU` solvers and the `NO_PRECONDITION` preconditioner. The default is the same as SLEPc's default.

```
subroutine pdecoefs(x,y,cxx,cxy,cyy,cx,cy,c,rs)
use phaml
real(my_real), intent(in) :: x,y
real(my_real), intent(out), dimension(:,:) :: cxx,cxy,cyy,cx,cy,c
real(my_real), intent(out), dimension(:) :: rs

cxx(1,1) = 1.0_my_real;  cxx(1,2) = 0.0_my_real
cxx(2,1) = 0.0_my_real;  cxx(2,2) = 1.0_my_real

cyy(1,1) = 1.0_my_real;  cyy(1,2) = 0.0_my_real
cyy(2,1) = 0.0_my_real;  cyy(2,2) = 1.0_my_real

  c(1,1) = 0.0_my_real;    c(1,2) = 1.0_my_real
  c(2,1) = 1.0_my_real;    c(2,2) = 0.0_my_real


rs(1) = -(2.0_my_real*exp(x-y) - (x+y)**4/8.0_my_real)
rs(2) = -(3.0_my_real*(x+y)**2 - exp(x-y))

cxy=0
cx=0
cy=0
end subroutine pdecoefs
```

Figure 4.1: `pdecoefs` for a coupled system.

4.2 Coupled Systems or Multicomponent Solutions

PHAML provides for the solution of certain types of coupled systems of elliptic PDEs, either boundary value problems or eigenvalue problems. These problems are also referred to as multicomponent problems if you prefer to think of it as a vector equation, rather than a system of equations, with a multicomponent solution, rather than multiple solutions. For these problems, Equations 1.1 - 1.3 are the same except the functions c_{xx}, c_{xy}, c_{yy}, c_x, c_y, c_u and c_{bc} are $n \times n$ arrays and the functions u, f and g are vectors of length n, where n is the number of equations in the coupled system. An example of subroutine `pdecoefs` for a coupled system is given in Figure 4.1 for the equations

$$\begin{aligned} -\nabla^2 u + v &= f_1 \\ -\nabla^2 v + u &= f_2 \end{aligned}$$

The number of equations is specified by the argument `system_size` to subroutine `phaml_create`. Subroutines `phaml_evaluate`, `phaml_evaluate_old`, `phaml_integrate`, phaml_query, and phaml_scale take an optional integer argument comp which specifies which component to use.

If any of the matrices c_{xx}, c_{yy}, c_u or c_{bc} is nonsymmetric, or c_{xy}, c_x or c_y is nonzero, then you must use a nonsymmetric solver like LAPACK_INDEFINITE_SOLVER (single processor only) or a nonsymmetric solver from PETSC, including PETSC_MUMPS_GEN_SOLVER and PETSC_SUPERLU_SOLVER, if so configured. Do not use the built-in hierarchical basis multigrid method (the default) as a solver or as a preconditioner.

4.3 Parabolic, Nonlinear, Etc. Problems

PHAML can be used to solve parabolic (time dependent) and nonlinear PDEs, but the user has to provide the iteration control in the main program. See the example examples/parabolic for an example of solving a time dependent parabolic problem using an implicit finite difference scheme in time, and examples/nonlinear for solving a nonlinear PDE using a simple Picard iteration.

The feature of PHAML that facilitates these problems is the storage of an "old" solution. You create an old solution with subroutine phaml_copy_soln_to_old (Section 6.4.3). This copies the current solution component of the phaml_solution_type variable to another component called the old solution. This would normally be done at the beginning or end of each iteration. To use the old solution, call phaml_evaluate_old (Section 6.4.8). You can evaluate the solution and/or the first derivatives and/or the second derivatives. This would normally be called from subroutine pdecoefs.

PHAML only provides for saving one "old" solution. You would think this would prohibit the use of methods that require more than one old solution. However, in many cases such problems can be reformulated as a coupled system of equations. See examples/waveeq for an example of solving a problem with a second order time derivative, which requires two old solutions, as a coupled system of two first order equations. An example of a second order backward difference scheme, which requires two old solutions, implemented as a coupled system of two equations is given in examples/bdf2. And examples/irk4 contains a fourth order 6-stage implicit Runge Kutta method implemented as a coupled system of six equations.

A time dependent problem requires setting an initial condition to start the solution. Similarly, a nonlinear problem requires an initial guess of the solution. These initial functions are set by calling phaml_solve_pde with task=SET_INITIAL and an appropriate termination criterion. The solution will be set to be the function in subroutine iconds (Section 6.3.5). It should then be copied to the old solution before starting the iteration.

If the solution does not change very much from one time step (or iteration) to the next, it may be possible to take several steps without changing the grid. In this case, the matrix does not change from one step to the next (provided the differential operator is linear). By default, PHAML destroys the linear system before returning from phaml_solve_pde. Setting the parameter `keep_linear_system=.true.` prevents this destruction so the matrix can be reused in the next call to `phaml_solve_pde` without recomputing it. Since the right hand side is likely to change, it is always recomputed. If the grid changes through refinement or load balancing, the kept linear system is automatically destroyed and recomputed. Also, the kept linear system is destroyed in `phaml_destroy`. See `examples/keeplinsys` for an example of how to use this feature.

4.4 3D Problems

The 3D version of PHAML does not support these features:

- next3p, hp bigger errind, refsoln edge, and refsoln elem *hp*-adaptive strategies
- local problem h and equilibrated residual error indicator
- multigrid, CG and GMRES native solvers
- native multigrid preconditioner
- MPI parallelism
- OpenMP parallelism

Except for those unsupported features, the 3D version of PHAML works exactly like the 2D version, with a few minor differences to handle the third dimension. The 3D version of the differential equation 1.1 is

$$-\frac{\partial}{\partial x}\left(c_{xx}\frac{\partial u}{\partial x}\right) - \frac{\partial}{\partial y}\left(c_{yy}\frac{\partial u}{\partial y}\right) - \frac{\partial}{\partial z}\left(c_{zz}\frac{\partial u}{\partial z}\right) - \frac{\partial}{\partial x}\left(c_{xy}\frac{\partial u}{\partial y}\right) - \frac{\partial}{\partial x}\left(c_{xz}\frac{\partial u}{\partial z}\right)$$
$$-\frac{\partial}{\partial y}\left(c_{yz}\frac{\partial u}{\partial z}\right) + c_x\frac{\partial u}{\partial x} + c_y\frac{\partial u}{\partial y} + c_z\frac{\partial u}{\partial z} + c_u u = f \quad \text{in } \Omega$$

The 2D and 3D versions of PHAML use common source code for most of the source files, with runtime selection of code sections that differ depending on the dimensionality. But there are a few files that have 2D and 3D versions, like the grid data structure module, and are selected at compile time. Thus PHAML is compiled for either 2D or 3D problems, but not both. To compile for 3D, use `tetrahedron` or `tetrahedron_fixdeg` for `PHAML_ELEMENT` when running `mkmkfile.sh`. `tetrahedron_fixdeg` will use a data structure with a fixed polynomial degree for the solution, and will save a considerable amount of memory when using *h*-refinement or *hp*-adaptive refinement with a small limit on the degree, as given by the argument `max_deg` of subroutine `phaml_solve_pde`. For *p*-refinement and *hp*-adaptive refinement with a large limit on the degree, use `tetrahedron`, in which the size of the solution component varies with the degree of the element.

The differences in the user interface for 3D are:

- Subroutine `pdecoefs` has additional arguments for the third dimension. The type specification for these arguments, and how they fit into the definition of the 3D PDE should be obvious from the 2D routine in Section 6.3.6. The argument list is `x,y,z,cxx,cyy,czz,cxy,cxz,cyz,cx,cy,cz,c,rs`.

- Subroutines `bconds, trues, truexs, trueys, phaml_integral_kernel` and `regularity` have an argument `z` that follows `x,y`.

- An additional subroutine `truezs` must be supplied, in the same manner as `truexs`.

- Subroutines `boundary_point, boundary_npiece` and `boundary_param` are not needed.

- Default values of some input parameters are different. See the Reference Manual 6.4.15.

There are also many differences in the graphics menu. You are encouraged to experiment with it.

`triangle_files` in `phaml_create` is still used to define the initial grid, but the input formats are different than the one used in 2D. For 3D, PHAML uses files in the formats of the 3D mesh generator Gmsh [19, 20]. There are two types of files used by PHAML: geometry files with a `geo` suffix, and mesh files with a `msh` suffix. One normally defines the domain and boundary markers (to be passed to `bcond`, see Section 6.3.1) in a geometry file. A mesh file is usually created by applying Gmsh to a geometry file. There are examples of both types of files in `examples/domains3D`. For a full description of these file types, see the Gmsh reference manual at `http://geuz.org/gmsh`. The character string in `triangle_files` can take one of three forms. If it is *filename*`.msh` then the given *filename* with `msh` suffix is a mesh file. Mesh files can only be used for domains with planar faces and straight line edges, because geometry information is required to properly refine curved boundary edges. If it is *filename*`.geo` then the file is a geometry file. PHAML will run Gmsh, putting the output in `phaml_`*filename*`.msh`. If it is *filename*`.geomsh` then both the geometry file *filename*`.geo` and mesh file *filename*`.msh` exist and the mesh file was created from the geometry file. (Note that `.geomsh` is not the suffix of a file name.) PHAML will use the mesh file to generate the initial grid and the geometry file when refining curved boundary edges. The default value for `triangle_files` is domain.msh.

PHAML supports a limited form of Gmsh's geometry files. It allows domains that have edges that are straight line segments, circle arcs, or ellipse arcs, and faces that are planar with an arbitrary number of edges, or a ruled surface with 3 or 4 edges. Planar faces can have holes. In general, a ruled surface is defined by transfinite interpolation of the edges. The exception is that if all the edges of a ruled surface are circle arcs with the same center, Gmsh has a hack to make that surface a segment of a sphere. The following features of a geometry file are supported:

- C and C++ style comments
- numeric expressions involving numbers (integer, fixed point, and exponential with e, E, d or D), variables, parentheses, and the operators +, -, *, /, ^and %.
- *variable* = *expression*
- Include
- geometry commands: Point, Physical Point, Circle, Ellipse, Line, Physical Line, Line Loop, Plane Surface, Ruled Surface (Gmsh before 3.0.0), Surface (Gmsh 3.0.0 and later), Physical Surface, Volume, and Physical Volume

It does not support character expressions, operators not listed above, built-in functions (Log, Sin, etc.), user-defined functions, loops and conditionals, predefined expression identifiers (Pi, newp, etc.), general commands not listed above, Spline, BSpline, Compound Line, Compound Surface, the "In Sphere" clause of a Ruled Surface or Surface statement, extrusions, transformations and mesh commands. Also, an expression cannot be split over more than one line and cannot contain an embedded comment. For an Include statement, the *char-expression* must be a string enclosed in double quotes which gives a file name that can be passed to a Fortran OPEN statement. A ruled surface can only have one line loop, i.e. no holes. Note that most unsupported features are simply ignored, which may or may not produce the desired effect, but some might cause the parser to fail.

Objects (vertices, edges, faces) on the boundary have an associated boundary marker, which can be used in subroutine `bconds` to determine which boundary condition to return. The boundary markers are defined by "Physical" objects in geometry files, and tags in mesh files. For example, a geometry file could define vertex 2 as a point at the origin by
`Point(2) = {0,0,0};`
and then define a physical point by
`Physical Point(5) = {2};`.
Here 2 is the point index; 5 is the index of the physical point and will be the boundary marker for that point. When Gmsh processes the geometry file to create a mesh file, it will create an "element" for that physical point with 5 as the first tag and an indication it is vertex 2.

It is recommended that you assign a nonzero boundary marker (zero is used to indicate interior objects) to every boundary object, unless your boundary conditions are defined by a single equation so that you don't need boundary markers. However, if there are boundary objects that do not appear in the mesh file as a Physical object or do not have tags, PHAML will assign a default boundary marker to it. The default boundary marker is the smallest positive integer that does not appear in the mesh file as a first tag. Boundary markers are assigned as follows:

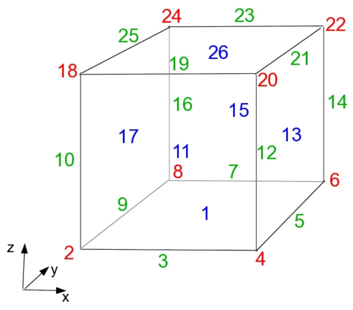


Figure 4.2: Assignment of boundary markers in `unitcube.msh`

- The boundary marker is set to 0 for interior vertices, edges and faces.
- If a boundary vertex, edge or face is in the mesh file with tags, the first tag is used as the boundary marker. By Gmsh's default, this is the index of the physical region containing the entity.
- If a boundary face is not in the mesh file or has no tags, it is assigned the default boundary marker.
- If a boundary edge is not in the mesh file or has no tags, it is assigned the boundary marker of one of the two faces that share the edge. If one of the faces has the default boundary marker, the edge gets the boundary marker of the other face (which could be the default boundary marker). Otherwise, if one face has Dirichlet boundary conditions and the other does not, the edge gets the boundary marker of the Dirichlet face. Otherwise, it gets the smaller of the two boundary markers.
- If a boundary vertex is not in the mesh file or has no tags, it is assigned the boundary marker of one of the edges that contains it. If any edges have Dirichlet boundary conditions, it is assigned the smallest boundary marker of those edges. Otherwise, it is assigned the smallest boundary marker of all the edges.

If you are solving a problem on the unit cube, you can use `examples3D/domains/unitcube.msh` as your mesh file. You might want to rename it `domain.msh`, which is the default value for `triangle_files`. Figure 4.2 shows the boundary markers for this mesh. Vertex boundary markers are shown in red, edge boundary markers in green, and face boundary markers in blue. For a more general parallelepiped, use `examples3D/domains/parpipe.geo`.

Periodic boundary conditions are supported only for parallelepipeds with faces parallel to the axes. They can be periodic in x, periodic in y and/or periodic in z. Since it is known what the matching periodic side is, you do not need to use the matching positive/negative boundary markers as in 2D, but you must indicate both sides are `PERIODIC` in subroutine `bconds`. Boundary edges and vertices that are at the intersection of a periodic side and a nonperiodic side can set the boundary condition type to either `PERIODIC` or whatever the type is on the nonperiodic side.

Chapter 5

Examples

Several examples of using PHAML are provided in directory `phaml-x.x.x/examples`. These can be used as tutorials to understand how PHAML works, or as templates for starting the implementation of your application. Depending on your set up, you might have to edit `master.f90` (or `spmd.f90` if you are using the SPMD model) slightly before running them, to change the termination criterion, number of processors, graphics choice, etc. The examples include:

`simple` – a trivial program that should be the first one you try.

`elliptic` – contains several linear scalar elliptic boundary value problems selected by a case statement.

`rectangle` – defines a rectangular domain with an $N \times M$ grid by writing a Triangle `.poly` file.

`L-domain` – the classic L shaped domain with a singular solution commonly used for testing adaptive refinement codes.

`domains` – contains several domains defined by Triangle `.poly` files.

`curved` – defines a domain with curved boundaries.

`holes` – defines a domain with holes.

`periodic` – periodic boundary conditions.

`eigenvalue` – an elliptic eigenvalue problem.

`parabolic` – solves a time-dependent parabolic PDE by an implicit finite difference scheme in t.

`keeplinsys` – solves a parabolic PDE without recomputing the matrix at every time step.

`nonlinear` – solves a nonlinear equation by Picard iteration.

`system` – solves a coupled system of 2 elliptic PDEs.

`all` – illustrates the use of all of the `phaml_*` routines.

`runtimepde` – determine user provided routines at run time

`waveeq` – solves the second order wave equations as a coupled system of two first order equations.

`bdf2` – solves a parabolic PDE by second order backward differences implemented as a coupled system of two equations.

`irk4` – solves a parabolic PDE by a 4^{th} order, 6-stage implicit Runge Kutta method implemented as a coupled system of six equations.

3D examples are in `phaml-x.x.x/examples3D`:

`simple` – a trivial program for a 3D problem.

`elliptic` – several 3D elliptic boundary value problems.

`eigenvalue` – a 3D eigenvalue problem.

`domains` – domains defined by Gmsh `.geo` and `.msh` files.

`periodic` – periodic boundary conditions.

There are also several programs under the `testdir` and `testdir3D` directories, but they do not contain comments to help you understand them.

Chapter 6

Reference Manual

6.1 Quick Start

This section provides a minimum of information about getting PHAML up and running the example programs. For many people, this will be sufficient to get started using PHAML with your application, as many applications may be implemented by modifying one of the examples. If you encounter problems, refer to the appropriate section of the User's Guide for further details. Also read the remainder of the User's Guide for a better understanding of how PHAML works and what options may be useful to you.

The four steps in getting started with PHAML are

1. obtaining the software,
2. compiling the PHAML library,
3. compiling an example, and
4. running the example.

For this brief tutorial, we will build and run the `simple` example as a master/slave message passing MPI program with the master spawning the slave processes, and without graphics.

6.1.1 Obtaining the software

PHAML can be obtained from the PHAML web page `http://math.nist.gov/phaml` by following the Software link. It comes as a gzipped tar file for Unix-like systems. (It has not yet been tested on MS Windows systems, but since it is written in standard Fortran 90, the adventurous may find that it works on MS Windows, too.) When unpacked, it will place everything in a new directory called `phaml-x.x.x`, where `x.x.x` is the current version number.

PHAML requires the BLAS and LAPACK libraries. You will probably find these are already installed on your computer, but if not, see Section 2.1.3.

For parallelism, you need an MPI library. You will probably find that Open MPI, LAM, MPICH, or a commercial MPI library is already installed on your computer, but if not see Section 2.1.4.

6.1.2 Compiling the PHAML library

The first step in compiling the PHAML library is to create the `Makefile`. This is done with the shell script `mkmkfile.sh` in the top PHAML directory. Since PHAML allows so many options in terms of what compilers and libraries to use, it would be difficult to auto-locate these files. So, you must modify `mkmkfile.sh` to specify some paths, command names, and defaults for your computer system. Instructions for modifying it can be found within the file.

Now create the `Makefile` with

```
./mkmkfile.sh PARALLEL messpass_spawn PARLIB mpi GRAPHICS none
```

You should replace `mpi` with `mpich`, `mpich2`, `openmpi`, or `lam` if you use an MPICH, Open MPI, or LAM library. You may omit some of the arguments if your defaults are already set to these values; defaults can be determined with `mkmkfiles.sh help`.

`make` should now compile the library and place it in the `lib` subdirectory.

6.1.3 Compiling an Example

Go to the directory `examples/simple` and type `make`. (The `Makefile`s for the examples were also created by `mkmkfile.sh`.) This should create the executables `phaml` and `phaml_slave`.

6.1.4 Running the Example

The details of running an MPI program vary with the different MPI libraries. You may need to check your MPI documentation to find the correct command(s). It may also require starting some daemon before running the execution command.

Note that you should specify *one* process, because you are running the master processes which will spawn the slave processes. The number of slaves is specified in the main program, `master.f90`.

If you are using LAM, try

```
lamboot
mpirun -np 1 phaml
```

If you are using MPICH, try

```
mpirun -np 1 phaml
```

If you are using MPICH2, try

```
mpiexec -n 1 phaml
```

If you are using Open MPI, try

```
mpiexec -np 1 phaml
```

6.1.5 Now what?

If you have successfully run the first example, you are ready to install the graphics and any other optional software you desire (Section 2.1), run the other examples, and begin working on your own application!

6.2 Public Entities in PHAML

The statement `use phaml` in a program unit provides access to the public entities in PHAML. These consist of a derived type, variables for the user to use, symbolic constants, and procedures. The procedures are described in Section 6.4. The other entities are described in this section.

6.2.1 phaml_solution_type

`phaml_solution_type` is a type that contains all the data used for solving the PDE (grid, etc.). The type is public, but the contents are private. You can declare one or more variables of this type and pass them to the PHAML procedures.

6.2.2 my_real

`my_real` is a symbolic constant that determines the kind of real numbers used in PHAML. This is defined in `global.f90`. You can change that definition there to select the kind to use, either single or double precision. Other kinds of real, if supported by your Fortran compiler, are not supported by PHAML because of the reliance on BLAS and LAPACK routines, which only come in single and double precision. Currently `my_real` is set for default double precision. To be sure that your program is using the same `kind` values, you should declare your variables as `real(kind=my_real)` and attach the kind to constants, e.g. `0.0_my_real`.

6.2.3 pde and my_pde_id

`pde` is a rank 1 allocatable array of type `phaml_solution_type`. If you are going to use more than one pde and they must communicate with each other, then you must use this array for your `phaml_solution` variables. It must be allocated before using `phaml_create`, and should be deallocated when you are done with it.

`my_pde_id` is an identifier for which pde a `phaml_solution` is associated with, usually the index into the array `pde` described above. It is usually used as the case statement variable in the user provided routines that define the PDE and boundary conditions.

See `examples/system_ss` for an example of the use of `pde` and `my_pde_id`. However, having multiple `phaml_solution_type` variables communicate with each other is very slow, so use of this capability is discouraged.

6.2.4 symbolic constants

Except for `my_real`, the symbolic constants are used as values for the arguments of the procedures. In this document and in the PHAML source code they are written in capital letters, but Fortran is not case sensitive so this is not necessary. They are defined as they arise in the description of the PHAML procedures. You can find a list of them by looking at the `public` statements at the beginning of `phaml.f90`. If you have a problem with one of the names conflicting with an entity in your code, you can use Fortran's renaming capability to circumvent it, for example

```
   use phaml, MY_EVAL_NAME => EIGENVALUE
```

6.3 User Provided Routines

The specifics of the problem to be solved are defined through a set of external subroutines that the user must provide. They must be external subroutines (i.e., not module or internal subroutines) because these are called from within PHAML and are compiled after the PHAML library has been built. They should contain a `use phaml` statement to get access to `my_real` and possibly other entities from PHAML.

This section describes the purpose of each of these routines and defines the interface of each. Also see `pde.f90` in each subdirectory of the PHAML `examples` directory for examples of these routines.

6.3.1 bconds

Subroutine `bconds` returns the boundary conditions at a given point. At each point, the boundary conditions are of the form

$$u = g$$

or

$$\left(c_{xx}\frac{\partial u}{\partial x} + c_{xy}\frac{\partial u}{\partial y}\right)\frac{\partial y}{\partial s} - c_{yy}\frac{\partial u}{\partial y}\frac{\partial x}{\partial s} + c_{bc}u = g$$

as described in Section 3.2.2.

```
   subroutine bconds(x,y,bmark,itype,c,rs)
```

`real(my_real), intent(in) ::` `x,y` – the point at which to evaluate the boundary conditions.

`integer, intent(in) ::` `bmark` – the boundary marker assigned in the Triangle data files.

`integer, intent(out) ::` `itype(:)` – the type of boundary condition at this point, given by symbolic constants from `module phaml`. It must be one of `DIRICHLET` (the first form above), `NATURAL` (the second form with c identically 0.0), or `MIXED` (the second form with c nonzero). The dimension of `itype` is `system_size`. The i^{th} value is the type of boundary condition for the i^{th} component.

`real(my_real), intent(out) :: c(:,:)` – the function c_{bc} in the boundary condition. The dimension is `system_size` by `system_size`. The $(i,j)^{th}$ entry is the coefficient of the j^{th} component in the boundary condition for the i^{th} component.

`real(my_real), intent(out) :: rs(:)` – the function g in the boundary condition. The dimension is `system_size`. The i^{th} entry is the right side of the boundary condition for the i^{th} component.

6.3.2 boundary_point

Subroutine `boundary_point` defines the boundary of the domain, if it is given by subroutines rather than triangle data files.

```
subroutine boundary_point(ipiece,s,x,y)
```

`integer, intent(in) :: ipiece` – the piece of the boundary from which to return a point.

`real(my_real), intent(in) :: s` – the parameter for the point to be determined.

`real(my_real), intent(out) :: x,y` – the point $(x(s),y(s))$ on piece `ipiece` of the boundary.

6.3.3 boundary_npiece

If the boundary of the domain is defined by the boundary subroutines, function `boundary_npiece` returns the number of boundary pieces in the definition. If the domain is defined by triangle data files, it returns 0 or a negative number. If the domain contains holes, it returns the number of pieces in the requested hole.

```
function boundary_npiece(hole)
```

`integer, intent(in) :: hole` – the hole for which to return the number of pieces, or 0 for the outer boundary. Holes are numbered consecutively starting with 1.

`integer :: boundary_npiece` – the number of boundary pieces in the requested hole or in the outer boundary if hole is 0.

6.3.4 boundary_param

Subroutine `boundary_param` gives the range of parameter values for each boundary piece.

```
subroutine boundary_param(start,finish)
```

`real(my_real), intent(out) :: start(:), finish(:)` – `start(i)` and `finish(i)` are the beginning and ending parameter values for the `i`th piece of the boundary, `i=1,number of boundary pieces`.

6.3.5 iconds

Subroutine `iconds` is used for setting the solution to a given function. For example, it can used for initial conditions for a time dependent problem or the initial guess for a nonlinear problem.

```
function iconds(x,y,comp,eigen)
```

`real(my_real), intent(in) :: x,y` – the point at which to evaluate the function.

`integer, intent(in) :: comp` – for multicomponent solutions, which component to return.

`integer, intent(in) :: eigen` – for eigenvalue problems in which more than one eigenvalue is computed, which eigenfunction to return.

`real(my_real) :: iconds` – the function value.

6.3.6 pdecoefs

Subroutine `pdecoefs` returns the values of the PDE coefficient functions and right side. The PDE is given by

$$-\frac{\partial}{\partial x}\left(c_{xx}\frac{\partial u}{\partial x}\right)-\frac{\partial}{\partial x}\left(c_{xy}\frac{\partial u}{\partial y}\right)-\frac{\partial}{\partial y}\left(c_{yy}\frac{\partial u}{\partial y}\right)+c_x\frac{\partial u}{\partial x}+c_y\frac{\partial u}{\partial y}+c_u u=f \quad \text{in } \Omega$$

as described in Section 3.2.1.

```
subroutine pdecoefs(x,y,cxx,cxy,cyy,cx,cy,c,rs)
```

`real(my_real), intent(in) :: x,y` – the point at which to evaluate the PDE.

`real(my_real), intent(out) :: cxx(:,:), cxy(:,:), cyy(:,:), cx(:,:), cy(:,:), c(:,:)` – the functions c_{xx}, c_{xy}, c_{yy}, c_x, c_y and c_u respectively. The dimension is `system_size` by `system_size`. The $(i,j)^{th}$ entry is the coefficient of the j^{th} component in the PDE for the i^{th} component.

`real(my_real), intent(out) :: rs(:)` – the function f. The dimension is `system_size`. The i^{th} value is the right side of the PDE for the i^{th} component.

6.3.7 phaml_integral_kernel

Subroutine `phaml_integrate` described in Sections 3.6.6 and 6.4.9 computes functionals of the computed solution of the form

$$\iint\limits_{\Omega} k(x,y)\ u_i^p(x,y)\ u_j^q(x,y)\ dx\ dy$$

where k is a kernel function defined in `phaml_integral_kernel`. In addition to a point at which to evaluate the kernel, the function takes an integer, `kernel`, which allows for the definition of several kernel functions in the same subroutine.

`function phaml_integral_kernel(kernel,x,y)`

`integer, intent(in) ::` `kernel` – an integer passed through `phaml_integrate` to allow a choice of different kernels.

`real(my_real), intent(in) ::` `x,y` – the point at which to evaluate the kernel.

`real(my_real) ::` `phaml_integral_kernel` – the kernel value, $k(x,y)$.

6.3.8 regularity

One strategy for *hp*-adaptive refinement is to provide *a priori* knowledge about the singular nature of the solution. Then h refinement is done near singularities and p refinement is done where the solution is smooth. This strategy is selected with `HP_APRIORI`, and the function `regularity` provides the user's *a priori* knowledge.

In theory, this routine should return the largest value of m such that the solution is in $H^m(T)$, i.e. the derivatives up to order m are in L^2, where T is the triangle whose vertices are given as input to the function. For multicomponent solutions, it should return the worst (i.e. smallest) such m among the components.

In practice, it can be used to guide refinement in other *a priori* known trouble areas, such as sharp peaks, boundary layers and wave fronts. The actual use is that p refinement is performed if the current degree of the triangle is less than the returned value, and h refinement is performed otherwise. So, for example, if you know some region contains a boundary layer, you could return 3.1 for any triangle that intersects that region to perform h-refinement with cubic elements over the boundary layer.

`function regularity(x,y)`

`real(my_real), intent(in) ::` `x(3),y(3)` – the x and y coordinates of the three vertices of the triangle.

`real(my_real) ::` `regularity` – the returned regularity.

6.3.9 trues

If the true solution of the PDE is known, you can provide it in function `trues`. This is used for printing norms of the error and for graphical display of the error and true solution. If you do not know the true solution, returning `huge(0.0_my_real)` will prevent printing and plotting of a bogus error.

```
function trues(x,y,comp,eigen)
```

`real(my_real), intent(in) :: x,y` – the point at which to evaluate the true solution

`integer, intent(in) :: comp` – for multicomponent solutions, which component to return.

`integer, intent(in) :: eigen` – for eigenvalue problems in which more than one eigenvalue is computed, which eigenfunction to return.

`real(my_real) :: trues` – the return value.

6.3.10 truexs

If the true solution of the PDE is known, you can provide the x derivative of it in function `truexs`. This is used for printing the energy norm, H^1 norm, and H^1 semi-norm of the error. If `trues` does not return `huge(0.0_my_real)` and you request the energy norm of the error, then you must provide the x derivative of the true solution in `truexs` or an incorrect value of these norms of the error will be printed.

```
function truexs(x,y,comp,eigen)
```

`real(my_real), intent(in) :: x,y` – the point at which to evaluate the x derivative of the true solution

`integer, intent(in) :: comp` – for multicomponent solutions, which component to return.

`integer, intent(in) :: eigen` – for eigenvalue problems in which more than one eigenvalue is computed, which eigenfunction to return.

`real(my_real) :: truexs` – the return value.

6.3.11 trueys

If the true solution of the PDE is known, you can provide the y derivative of it in function `trueys`. This is used for printing the energy norm, H^1 norm, and H^1 semi-norm of the error. If `trues` does not return `huge(0.0_my_real)` and you request the energy norm of the error, then you must provide the y derivative of the true solution in `trueys` or an incorrect value of these norms of the error will be printed.

```
function trueys(x,y,comp,eigen)
```

`real(my_real), intent(in) ::` `x,y` – the point at which to evaluate the y derivative of the true solution

`integer, intent(in) ::` `comp` – for multicomponent solutions, which component to return.

`integer, intent(in) ::` `eigen` – for eigenvalue problems in which more than one eigenvalue is computed, which eigenfunction to return.

`real(my_real) ::` `trueys` – the return value.

6.3.12 update_usermod

The application can include a module called `phaml_user_mod` to provide access to global variables in the user provided subroutines. However, values assigned to these variables in the main program are only available in the master process. Subroutine `update_usermod` passes the current value of these variables from the master to the slaves. For an example use of this facility, see `examples/parabolic` where it is used to pass the time step to the slaves. A working version of this subroutine is shown in Figure 6.1, or can be copied from `examples/parabolic/pde.f90`. In the example, the `integer` variable `ivar` and the `real(my_real)` variables `rvar1` and `rvar2` are declared in `module phaml_user_mod`. If you do not use this facility, you can copy a dummy version of the subroutine from `examples/simple/pde.f90`.

6.4 PHAML procedures

6.4.1 phaml_compress

`phaml_compress` compresses the `phaml_solution_type` data by moving all the unused elements, edges and vertices after the used ones. If considerable derefinement has occurred, this can significantly reduce the size of files created by `phaml_store`.

```
subroutine phaml_compress(phaml_solution)
```

`type(phaml_solution_type), intent(inout) ::` `phaml_solution` – the solution to compress.

6.4.2 phaml_connect

`phaml_connect` connects two `phaml_solution_type` variables so they can communicate. If one will request that another evaluate its solution, then they must be connected. See `examples/system_ss` and Section 6.2.3. However, having multiple `phaml_solution_type` variables communicate with each other is very slow, so use of this capability is discouraged.

```
subroutine phaml_connect(pde1, pde2)
subroutine update_usermod(phaml_solution)

!----------------------------------------------------
! This routine updates the module variables on the slave processes by
! sending them from the master process
!----------------------------------------------------

use phaml
use phaml_user_mod

!----------------------------------------------------
! Dummy arguments

type(phaml_solution_type), intent(in) :: phaml_solution

!----------------------------------------------------
! Local variables:

! Declare these arrays big enough to hold the variables to be sent

integer :: iparam(1)
real(my_real) :: rparam(2)

!----------------------------------------------------
! Begin executable code

! Copy the module variables into the arrays, putting integer variables
! into iparam and real variables into rparam.

   iparam(1) = ivar
   rparam(1) = rvar1
   rparam(2) = rvar2

! Call the routine that performs the actual exchange.  Don't change this line.

   call master_to_slaves(phaml_solution,iparam,rparam)

! Copy the arrays into the module variables, using the same correspondence
! between module variable and array index as was used above.

   ivar  = iparam(1)
   rvar1 = rparam(1)
   rvar2 = rparam(2)

end subroutine update_usermod
```

Figure 6.1: An example of subroutine update_usermod.

`integer, intent(in) :: pde1, pde2` – indices into the pde array in module phaml.

6.4.3 phaml_copy_soln_to_old

`phaml_copy_soln_to_old` makes a copy of the solution in `phaml_solution` which can be evaluated by `phaml_evaluate_old` (Section 6.4.8). The main purpose of this is to provide the "old" solution and derivatives for time stepping in time dependent problems and iterating in nonlinear problems.

```
subroutine phaml_copy_soln_to_old(phaml_solution)
```

`type(phaml_solution_type), intent(inout) :: phaml_solution` – the phaml solution in which to make a copy of the solution.

6.4.4 phaml_create

`phaml_create` creates a variable to contain a phaml_solution, i.e., it initializes the internals of a variable of type `phaml_solution_type`. It also spawns the associated slave and graphics processes. This should be called with each variable of type `phaml_solution_type` in your program.

All arguments except `phaml_solution` are optional.

```
   subroutine phaml_create(phaml_solution, nproc, nthread, draw_grid_who,
spawn_form, debug_command, display, graphics_host, output_unit, error_unit,
output_now, id, system_size, eq_type, max_blen, triangle_files, update_umod,
init_alloc)
```

`type (phaml_solution_type) phaml_solution` – the variable to initialize.

`integer nproc` – the number of processes working in parallel. The default is 1.

`integer nthread` – the number of OpenMP threads in each process. The default is whatever is set outside of PHAML, for example via OMP_NUM_THREADS.

`draw_grid_who` – which processes should display grid graphics. The grid graphics are not just the grid, but also the computed solution and many other useful displays. Valid values are:

- `MASTER` – the graphics process associated with the master process draws a grid that is a consolidation of the slave's grids.
- `SLAVES` – each slave has an associated graphics process, which draws the grid as known to that slave. Note that there will be a graphics window for each slave.
- `EVERYONE` – both MASTER and SLAVES.
- `NO_ONE` – no graphics are drawn.

The default is `NO_ONE`.

`spawn_form` – whether or not to provide debugging capability with spawned processes. An xterm running the slave under the debugger given by `debug_command` is brought up. Valid values are:

- `NORMAL_SPAWN` – no debugging.
- `DEBUG_SLAVE` – spawn the slave processes under the debugger.
- `DEBUG_GRAPHICS` – spawn the graphics processes under the debugger.
- `DEBUG_BOTH` – spawn both slaves and graphics under the debugger.

The default is `NORMAL_SPAWN`.

`character(len=*) debug_command` – the command name of the debugger to use in an xterm when `spawn_form` is not `NORMAL_SPAWN` and MPI is used. Limited to 64 characters. The default is `"gdb"`.

`character(len=*) display` – in some environments, the `-display` argument is needed for `xterm` when `spawn_form` is not `NORMAL_SPAWN`. This value is used for that argument. If it is `"default"` then the `-display` argument is not used for `xterm`. Limited to 64 characters. The default is `"default"`.

`character(len=*) graphics_host` – the name of the host on which to spawn the graphics processes. This is useful if you want to force the graphics processes to run on the workstation whose display is in front of you, or if you want graphics to run on a particular architecture. This is a “hint” which may be obeyed or ignored depending on the implementation of MPI.

`integer output_unit` – the unit number for printed output. It should either be a pre-connected unit (e.g. standard output) or be opened as `FORMATTED` with a call to `phaml_popen` immediately after `call phaml_create`. The default is 6.

`integer error_unit` – the unit number for error messages. It should either be a pre-connected unit (e.g. standard error) or be opened as `FORMATTED` with a call to `phaml_popen` immediately after `call phaml_create`. The default is 0.

`integer output_now` – since `output_unit` and `error_unit` may not be available until after `phaml_create` is complete, a unit must be provided for any output (i.e. error messages) that occurs from subroutine `phaml_create`. This should be a pre-connected unit. The default is 6.

`integer id` – an identifier for the PDE, simply for use by the user in subroutines `pdecoefs`, `bconds`, etc. It is available as `my_pde_id` in module `phaml`. See Section 6.2.3. The default is 0.

`integer system_size` – number of equations in a coupled system of PDEs, or equivalently, number of components in a multicomponent solution. The default is 1.

`integer eq_type` – type of equation to create. Valid values are:

> `ELLIPTIC` – solve an elliptic boundary value PDE.
>
> `EIGENVALUE` – solve an elliptic eigenvalue PDE.

The default is `ELLIPTIC`.

`real(my_real) max_blen` – maximum length of a boundary segment if the domain is defined by the boundary subroutines.

The default is ∞, defined to be `huge(0.0_my_real)`.

`character(len=*) triangle_files` – in 2D, the root name of the `.node`, `.ele`, `.neigh`, `.poly` and `.edge` triangle data files. If the domain is defined by triangle data files and the file names include Triangle's iteration number (usually `.1`), include the iteration number. If the domain is defined by the boundary subroutines, this is used as the root of the created triangle data files, and, if run MPI parallel, it must reside on a file system that is shared by all processes. In 3D, indicates the name of a .msh and/or .geo file to define the domain and initial grid (see Sect. 4.4)

The default is `"domain"` in 2D and `"domain.msh"` in 3D.

`logical update_umod` – run `update_usermod` as soon as the communication has been initialized. This is needed if `phaml_user_mod` has any parameters that affect the definition of the domain, or need to be set before the first solution on the initial grid.

The default is `.false.`

`integer init_alloc` – initially allocate the grid to be big enough for init_alloc vertices per processor. Using a number as large as possible will reduce the time spent in reallocation as the grid grows.

6.4.5 phaml_destroy

`phaml_destroy` destroys a variable of type `phaml_solution_type`, i.e., frees the memory contained in it. It also terminates the slave and graphics processes. If you have multiple `phaml_solution_type` variables that are not needed simultaneously, you should destroy those no longer needed before creating those not yet used, to reduce the possibility of running out of memory. Also, if a `phaml_solution_type` variable is used more than once and is to be recreated to give it a fresh start, it should be destroyed before being created again to avoid a memory leak.

```
subroutine phaml_destroy(phaml_solution, finalize_mpi)
```

`type (phaml_solution_type) phaml_solution` – the variable to destroy

`logical finalize_mpi` – if `.false.`, do not call `mpi_finalize` from the master. It should be `.true.` if and only if this is the last call to `phaml_destroy`.

The default is `.true.`

6.4.6 phaml_evaluate

`phaml_evaluate` evaluates the computed solution and/or derivatives of it at the given points.

`subroutine phaml_evaluate(phaml_solution, x, y, u, ux, uy, uxx, uyy, comp, eigen, z, uz, uzz)`

`type(phaml_solution_type), intent(in) :: phaml_solution` – the solution to evaluate.

`real(my_real), intent(in) :: x(:), y(:)` – array of x and y coordinates at which to evaluate the solution.

`real(my_real), intent(out), optional :: u(:), ux(:), uy(:), uxx(:), uyy(:)` – returned as the computed solution and derivatives at the given points. Those that are present determine what is evaluated. Must have `size(u) == size(x), etc.`

`integer, intent(in), optional :: comp` – for multicomponent solutions, which component to evaluate. The default is 1.

`integer, intent(in), optional :: eigen` – for eigenvalue problems, which eigenfunction to evaluate. The default is 1.

`real(my_real), intent(in), optional :: z(:)` – array of z coordinates at which to evaluate the solution. Must be present if and only if PHAML was compiled for 3D problems.

`real(my_real), intent(out), optional :: uz(:), uzz(:)` – returned as the derivatives at the given points. Those that are present determine what is evaluated. Must have `size(uz) == size(x), etc.`

6.4.7 phaml_get_grid_soln

`phaml_get_grid_soln` returns the vertices of the grid and the solution at those vertices.

`subroutine phaml_get_grid_soln(phaml_solution, x, y, u, comp, eigen, z)`

`type(phaml_solution_type), intent(in) :: phaml_solution` – the solution from which to get the grid and solution.

`real(my_real), pointer :: x(:), y(:), u(:)` – `x` and `y` are returned as the coordinates of the vertices of the triangles (tetrahedra in 3D) of the grid; `u` is the computed solution at those vertices. They should be disassociated on input and will be allocated to the correct size. You should deallocate them when done with them. To determine the number of points returned, use `size(x)`.

`integer, intent(in), optional :: comp` – for multicomponent solutions, which component to return. The default is 1.

`integer, intent(in), optional :: eigen` – for eigenvalue problems, which eigenfunction to return. The default is 1.

`real(my_real), pointer, optional :: z(:)` – returned as the z coordinates of the tetrahedra. Must be present if and only if PHAML was compiled for 3D problems.

6.4.8 phaml_evaluate_old

`phaml_evaluate_old` evaluates the "old" solution and/or derivatives at the given point(s). Unlike all the other phaml subroutines, it should not be called from the main program. It is intended to be called from the user routines that define the problem (`pdecoefs`, etc.) to provide the "old" solution and derivatives for time stepping in time dependent problems and iterating in nonlinear problems.

```
  subroutine phaml_evaluate_old(x, y, u, ux, uy, uxx, uyy, comp, eigen,
z, uz, uzz)
```

`real(my_real), intent(in) :: x, y` – x and y coordinates of the point at which to evaluate the solution.

`real(my_real), intent(out), optional :: u, ux, uy, uxx, uyy` – returned as the old solution, x derivative, y derivative, second x derivative and second y derivative at the given point. Any combination of the five may be present.

`integer, intent(in), optional :: comp` – for multicomponent solutions, which component to evaluate. The default is 1.

`integer, intent(in), optional :: eigen` – for eigenvalue problems, which eigenfunction to evaluate. The default is 1.

`real(my_real), intent(in), optional :: z` – z coordinate at which to evaluate the solution. Must be present if and only if PHAML was compiled for 3D problems.

`real(my_real), intent(out), optional :: uz, uzz` – returned as the first and second z derivative at the given point. May be present only if PHAML was compiled for 3D problems.

6.4.9 phaml_integrate

`phaml_integrate` returns a functional of the computed solution, i.e. an integral of a computed solution or product of two computed solutions or powers of computed solutions, weighted by a kernel function. It computes

$$\iint_{\Omega} k(x,y)\ u^{p}_{comp1,eigen1}(x,y)\ u^{q}_{comp2,eigen2}(x,y)\ dx\ dy$$

where k is a kernel function defined in `phaml_integral_kernel` (see Section 6.3.7).

`function phaml_integrate(phaml_solution, kernel, comp1, eigen1, comp2, eigen2, p, q)`

`type(phaml_solution_type), intent(in) :: phaml_solution` – the solution to integrate.

`integer, intent(in) :: kernel` – allows you to select among different kernel functions. It is passed to `phaml_integral_kernel` where it can be used, for example, in a case statement to determine the kernel to use.

`integer, intent(in), optional :: comp1, eigen1, comp2, eigen2` – which component(s) of a multicomponent solution and which eigenfunction(s) of an eigenvalue problem to use. All of them default to 1. If `comp1` is omitted then `comp2` must also be omitted, and likewise for `eigen1` and `eigen2`. If `comp2` and `eigen2` are both omitted, then $u_{comp2,eigen2}$ is omitted from the integral.

`integer, intent(in), optional :: p, q` – the powers to which to raise the computed solutions in the integral. The default is 1.

6.4.10 phaml_pclose

`phaml_pclose` closes unit number `unit` on all processors in `phaml_solution`. See also `phaml_popen` in Section 6.4.11.

`subroutine phaml_pclose(phaml_solution, unit)`

`type (phaml_solution_type), intent(in) :: phaml_solution` – the solution for which the files are being closed.

`integer, intent(in) :: unit` – the unit number to close.

6.4.11 phaml_popen

`phaml_popen` opens unit number `unit` on all processors in `phaml_solution`. If `file` is of the form "root.suffix" then the actual filenames are `rootXXXX.suffix` for processor number `XXXX`, where the number of digits in `XXXX` is the minimum needed for the number of processors in `phaml_solution`. The master processor is number 0. If there is no "." in `file`, then there is no suffix and `XXXX` is appended to the filename. The filename is limited to 1024 characters and the number of processors is limited to 9999. If the filename does not contain the full path, the location of the file is compiler dependent. Good places to look for it are the current working directory and the user's home directory.

```
   subroutine phaml_popen(phaml_solution, unit, file, form, iostat)
```

`type (phaml_solution_type), intent(in) :: phaml_solution` – the solution for which the files are being opened.

`integer, intent(in) :: unit` – unit number to open.

`character(len=*), intent(in) :: file` – base file name for the files.

`character(len=*), intent(in), optional :: form` – must take the value `"FORMATTED"` or `"UNFORMATTED"` to determine the type of file to open. Default is `"FORMATTED"`.

`integer, intent(out), optional :: iostat` – 0 if the file was successfully opened on all processors. -10 if `form` is present with a value other than `"FORMATTED"` or `"UNFORMATTED"`. -11 if `unit` is negative. Any other value is the value of `iostat` returned by the Fortran `OPEN` statement.

6.4.12 phaml_query

`phaml_query` returns values of interest about the grid and solution. All arguments except `phaml_solution`, `comp`, `eigen` and `error_estimator` are optional and `intent(out)`. Include those you wish to receive as keyword arguments. `phaml_solution` is mandatory and intent(in). `comp`, `eigen` and `error_estimator` are optional and intent(in).

```
   subroutine phaml_query(phaml_solution, nvert, nvert_proc, nvert_own,
nelem, nelem_proc, nelem_own, neq, neq_proc, neq_own, nlev, min_degree,
max_degree, linf_error, energy_error, h1_error, h1_seminorm_error, l2_error,
max_error_indicator, linf_error_estimate, energy_error_estimate, h1_error_estimate,
h1_seminorm_error_estimate, l2_error_estimate, linf_solution, l2_solution,
energy_solution, linf_u, l2_u, energy_u, h1_u, h1_seminorm_u, linf_true,
l2_true, energy_true, h1_true, h1_seminorm_true, eigenvalues, eigenvalue_error_estimate,
eigensolver_eval_errest, eigensolver_l2_residual, eigensolver_niter,
eigensolver_nconv, comp, eigen, error_estimator)
```

`type(phaml_solution_type) :: phaml_solution` – the solution to query

`integer :: nvert` – the number of vertices in the grid

`integer, dimension(nproc) :: nvert_proc` – the number of vertices in the grid of each processor

`integer, dimension(nproc) :: nvert_own` – the number of vertices owned by each processor `integer ::` `nelem` – the number of elements in the grid

`integer, dimension(nproc) ::` `nelem_proc` – the number of elements in the grid of each processor

`integer, dimension(nproc) ::` `nelem_own` – the number of elements owned by each processor

`integer ::` `neq` – the number of equations in the linear system

`integer, dimension(nproc) ::` `neq_proc` – the number of equations in the linear system of each processor

`integer, dimension(nproc) ::` `neq_own` – the number of equations owned by each processor

`integer ::` `nlev` – the number of levels of refinement

`integer ::` `min_degree` – the smallest polynomial degree of an element

`integer ::` `max_degree` – the largest polynomial degree of an element

`real(my_real) ::` `linf_error` – the L^∞ norm of the error (at the vertices and quadrature points of a sixth order quadrature rule), if the true solution is known

`real(my_real) ::` `energy_error` – the energy norm of the error (approximated by a sixth order quadrature rule), if the true solution and its derivatives are known

`real(my_real) ::` `h1_error` – the H^1 norm of the error (approximated by a sixth order quadrature rule), if the true solution and its derivatives are known

`real(my_real) ::` `h1_seminorm_error` – the H^1 semi-norm of the error (approximated by a sixth order quadrature rule), if the true solution and its derivatives are known

`real(my_real) ::` `l2_error` – the L^2 norm of the error (approximated by a sixth order quadrature rule), if the true solution is known

`real(my_real) ::` `max_error_indicator` – the largest error indicator

`real(my_real) ::` `linf_error_estimate` – an estimate of the L^∞ norm of the error

`real(my_real) ::` `energy_error_estimate` – an estimate of the energy norm of the error

`real(my_real) ::` `h1_error_estimate` – an estimate of the H^1 norm of the error `real(my_real) :: h1_seminorm_error_estimate` – an estimate of the H^1 semi-norm of the error

`real(my_real) :: l2_error_estimate` – an estimate of the L^2 norm of the error

`real(my_real) :: linf_solution` – the discrete ℓ^∞ norm of the solution vector

`real(my_real) :: l2_solution` – the discrete ℓ^2 norm of the solution vector

`real(my_real) :: energy_solution` – the discrete energy norm of the solution vector

`real(my_real) :: linf_u` – the continuous L^∞ norm of the solution, approximated using the vertices and the quadrature points of a sixth order quadrature rule

`real(my_real) :: l2_u` – the continuous L^2 norm of the solution, approximated with a sixth order quadrature rule

`real(my_real) :: energy_u` – the continuous energy norm of the solution, approximated with a sixth order quadrature rule

`real(my_real) :: h1_u` – the continuous H^1 norm of the solution, approximated with a sixth order quadrature rule

`real(my_real) :: h1_seminorm_u` – the continuous H^1 semi-norm of the solution, approximated with a sixth order quadrature rule

`real(my_real) :: linf_true` – the continuous L^∞ norm of the true solution, approximated using the vertices and the quadrature points of a sixth order quadrature rule

`real(my_real) :: l2_true` – the continuous L^2 norm of the true solution, approximated with a sixth order quadrature rule

`real(my_real) :: energy_true` – the continuous energy norm of the true solution, approximated with a sixth order quadrature rule

`real(my_real) :: h1_true` – the continuous H^1 norm of the true solution, approximated with a sixth order quadrature rule

`real(my_real) :: h1_seminorm_true` – the continuous H^1 semi-norm of the true solution, approximated with a sixth order quadrature rule

`real(my_real), dimension(num_eval) :: eigenvalues` – the computed eigenvalues, for eigenvalue problems

`real(my_real), dimension(num_eval) :: eigenvalue_error_estimate` – an estimate of the error in each eigenvalue in the continuous problem `real(my_real), dimension(num_eval) :: eigensolver_eval_errest` – an estimate of the error in each eigenvalue in the discrete eigenvalue problem

`real(my_real), dimension(num_eval) :: eigensolver_l2_residual` – the ℓ^2 norm of the residual of the discrete eigenvalue problem for each eigenpair

`integer :: eigensolver_niter` – number of iterations used by the eigensolver

`integer :: eigensolver_nconv` – number of converged eigenvalues

`integer :: comp` – for multicomponent solutions, which component to report. Energy and H^1 norms and H^1 semi-norms cover all components in a single norm. L^∞ and L^2 norms cover each component in individual norms. The default is 1.

`integer :: eigen` – for eigenvalue problems, which eigenfunction to report. The default is 1.

`integer :: error_estimator` – which error indicator to use for error estimates and error indicators. The default is EXPLICIT_ERRIND.

6.4.13 phaml_restore

`phaml_restore` restores information for `phaml_solution` from files created by subroutine `phaml_store` (see Section 6.4.16.

```
subroutine phaml_restore(phaml_solution, unit, do_draw_grid, pause)
```

`type (phaml_solution_type), intent(inout) :: phaml_solution` – the solution into which the data will be read. If `phaml_solution` was previously used, it should be destroyed first with `phaml_destroy` (see Section 6.4.5) to avoid a memory leak. Whether or not it was previously used, it must be created with `phaml_create` (see Section 6.4.4) before passing it to `phaml_restore`.

`integer, intent(in) :: unit` – the unit number to read from, which should have been opened with `phaml_popen` using the same form as was used when `phaml_store` created the files.

`logical, intent(in), optional :: do_draw_grid` – whether or not to draw the solution immediately after reading it.

`logical, intent(in), optional :: pause` – if `do_draw_grid` is true, whether or not to pause after drawing the grid.

6.4.14 phaml_scale

`phaml_scale` scales the computed solution by multiplying by `factor`.

```
   subroutine phaml_scale(phaml_solution, factor, comp, eigen)
```

`type(phaml_solution_type), intent(inout) :: phaml_solution` – the solution to scale.

`real(my_real), intent(in) :: factor` – the factor by which to multiply.

`integer, intent(in), optional :: comp` – for multicomponent solutions, which component to scale. The default is 1.

`integer, intent(in), optional :: eigen` – for eigenvalue problems, which eigenfunction to scale. The default is 1.

6.4.15 phaml_solve_pde

`phaml_solve_pde` solves the PDE. All arguments are optional, except `phaml_solution`, so you only need to provide those for which you do not want to take the default. All arguments are `intent(in)` except `phaml_solution` which is `intent(inout)` and `iterm` and `grid_modified` which are `intent(out)`. It is recommended that the call use keyword arguments for all arguments except possibly `phaml_solution`. Since there is such a large number of arguments to this routine, they are placed into subsections by category.

```
   subroutine phaml_solve_pde(phaml_solution, iterm, grid_modified,
max_elem, max_vert, max_eq, max_lev, max_deg, stop_on_maxlev, stop_on_maxdeg,
max_refsolveloop, min_elem_size, term_energy_err, term_Linf_err, term_L2_err,
term_H1_err, term_H1_seminorm_err, term_eigenvalue_err, task, print_grid_when,
print_grid_who, print_error_when, print_error_who, print_energy_norm_error,
print_H1_norm_error, print_H1_seminorm_error, print_Linf_norm_error, print_L2_norm_error,
print_energy_norm_errest, print_H1_norm_errest, print_H1_seminorm_errest,
print_Linf_norm_errest, print_L2_norm_errest, print_linsys_when, print_linsys_who,
print_solver_when, print_solver_who, print_time_when, print_time_who,
print_eval_when, print_eval_who, print_header_who, print_trailer_who,
print_warnings, clocks, draw_grid_when, pause_after_draw, pause_after_phases,
pause_at_start, pause_at_end, solve_init, keep_linear_system, sequential_vert,
inc_factor, error_estimator, errtype, reftype, refterm, reftol, reftol_factor,
coarsentol, coarsentol_factor, reftol_scale_energy, refmaxloop, recoarsen_limit,
recoarsen_tol, hp_strategy, t3s_gamma, t3s_eta, t3s_nunif, t3s_maxref,
t3s_maxdeginc, tp_gamma, sp_gamma_h, sp_gamma_p, pbias, hp_patch_mult,
hp_patch_add, derefine, partition_method, edge_rule, p_compatibility,
max_p_diff, zoltan_param_file, prebalance, postbalance, petsc_matrix_free,
solver, preconditioner, mg_cycles, mg_tol, mg_prerelax, mg_postrelax,
mg_prerelax_ho, mg_postrelax_ho, krylov_iter, krylov_restart, krylov_tol,
mg_comm, ignore_quad_err, eigensolver, num_eval, lambda0, st_shift, st_antishift,
```

harmonic_extraction, slepc_true_residual, scale_evec, eigen_ncv, eigen_maxit,
eigen_tol, degree, inc_quad_order, pde_has_first_order_terms, pde_has_cross_derivative,
laplacian_operator, isosceles_right_triangles, bc_changed, hypre_BoomerAMG_tol,
hypre_BoomerAMG_trunc_factor, hypre_BoomerAMG_strong_threshold, hypre_BoomerAMG_max_row_sum,
hypre_BoomerAMG_relax_weight, hypre_BoomerAMG_outer_relax_weight, hypre_BoomerAMG_cycle_type,
hypre_BoomerAMG_max_levels, hypre_BoomerAMG_max_iter, hypre_BoomerAMG_P_max_elmts,
hypre_BoomerAMG_agg_num_levels, hypre_BoomerAMG_agg_num_paths, hypre_BoomerAMG_num_sweeps_all,
hypre_BoomerAMG_num_sweeps_down, hypre_BoomerAMG_num_sweeps_up, hypre_BoomerAMG_num_sweeps_coar
hypre_BoomerAMG_relax_type_all, hypre_BoomerAMG_relax_type_down, hypre_BoomerAMG_relax_type_up,
hypre_BoomerAMG_relax_type_coarsest, hypre_BoomerAMG_relax_order, hypre_BoomerAMG_measure_type
hypre_BoomerAMG_coarsen_type, hypre_BoomerAMG_interp_type, hypre_BoomerAMG_print_statistics,
hypre_BoomerAMG_print_debug, hypre_Pilut_tol, hypre_Pilut_maxiter, hypre_Pilut_factorrowsize,
hypre_ParaSails_thresh, hypre_ParaSails_filter, hypre_ParaSails_loadbal,
hypre_ParaSails_nlevels, hypre_ParaSails_sym, hypre_ParaSails_logging,
hypre_ParaSails_reuse, petsc_richardson_damping_factor, petsc_chebychev_emin,
petsc_chebychev_emax, petsc_gmres_max_steps, petsc_rtol, petsc_atol,
petsc_dtol, petsc_maxits, petsc_ilu_levels, petsc_icc_levels, petsc_sor_omega,
petsc_sor_its, petsc_sor_lits, petsc_eisenstat_nodiagscaling, petsc_eisenstat_omega,
petsc_asm_overlap)

6.4.15.1 Miscellaneous arguments

`type (phaml_solution_type) phaml_solution` – the variable that contains the main data structures. It must be created by subroutine `phaml_create` before passing it to `phaml_solve_pde`.

`integer task` – what task to perform. Valid values are:

- `BALANCE_REFINE_SOLVE` – go through a loop repeatedly doing load balance, refinement and solution phases.
- `SET_INITIAL` – loop through the phases, but for the solution phase use interpolation of the function in `iconds`.
- `BALANCE_ONLY` – just do one load balancing phase.
- `REFINE_ONLY` – just do one refinement phase.
- `SOLVE_ONLY` – just do one solution phase.

The default is `BALANCE_REFINE_SOLVE`.

`logical solve_init` – determines whether or not to compute the solution on the initial grid. Sometimes you might not want to if the grid comes from a previous call.

The default is .true.

`logical keep_linear_system` – don't destroy the last linear system before returning.

The default is .false.

`logical pde_has_first_order_terms` – indicates whether or not one of c_x or c_y is not identically zero.

The default is .true. if either c_x or c_y is nonzero at the midpoint of one of the initial elements, and .false. otherwise.

`logical pde_has_cross_derivative` – indicates whether or not c_{xy} is not identically zero.

The default is .true. if c_{xy} is nonzero at the midpoint of one of the initial elements, and .false. otherwise.

`logical laplacian_operator` – indicates whether or not the PDE operator is the Laplacian, i.e. c_{xx} and c_{yy} are identically one while all other coefficients are identically zero (the right side can be anything).

The default is .true. if c_{xx} and c_{yy} are 1.0 at the midpoint of every initial element and c_{xy}, c_x, c_y and c are 0.0 at the midpoint of every initial element, and .false. otherwise.

`logical isosceles_right_triangles` – indicates whether or not every triangle in the initial grid is an isosceles right triangle with the peaks at the right angles.

The default is .true. if every initial triangle appears to be an isosceles right triangle with the right angle at the third vertex, within roundoff error, and .false. otherwise.

`bc_changed` – on calls after the first, setting this to false can save time if it is known that the boundary conditions and true solution (if provided) have not changed since the previous call.

The default is .true.

6.4.15.2 Termination arguments

`integer iterm` – termination code. If positive, a termination criterion was met. If negative, an error occurred. For the current meaning of the codes, see `global.f90` and look for the string `termination`.

`logical grid_modified` – True if and only if changes were made to the grid in this call, excluding changes in the solution value and load balancing.

`integer max_elem` – the maximum number of elements to use (termination criterion).

The default is ∞, defined to be `huge(0)`.

`integer max_vert` – maximum number of vertices to use (termination criterion).

The default is ∞, defined to be `huge(0)`.

`integer max_eq` – maximum number of equations in the linear system (a.k.a. degrees of freedom) to use (termination criterion).

The default is ∞, defined to be `huge(0)`.

`integer max_lev` – the maximum number of *h* refinement levels to use. If an element is flagged for *h* refinement and the number of levels would exceed `max_lev`, then the element is quietly not refined, except for some *hp* strategies where it is *p*-refined instead. The number of levels is also limited by the size of the hash keys, which is set at the time the PHAML library is compiled (see Section 2.2.1) and the number of element in the initial grid. For 32 bit integers and a very coarse initial grid the maximum is about 25-30 for `PHAML_HASHSIZE`=1 and 55-60 for `PHAML_HASHSIZE`=2. If *h* refinement would cause the hash to overflow, the element is quietly not refined, except for some *hp* strategies where it is *p*-refined instead.

The default is the largest number that prevents overflow in the hash keys.

`integer max_deg` – the maximum polynomial degree for the approximation space. If an element is flagged for *p* refinement and the degree would exceed `max_deg`, then the element is quietly not refined, except for some *hp* strategies where it is *h*-refined instead.

In most cases the default is 22, which corresponds to the maximum degree for which the currently implemented quadrature rules will give the exact solution if the solution is a polynomial of degree `max_deg`. If `reftype` is `HP_ADAPTIVE` and `hp_strategy` is `HP_NEXT3P`, the default is 19. Otherwise, if `error_estimator` is `LOCAL_PROBLEM_P` or `EQUILIBRATED_RESIDUAL`, or `reftype` is `HP_ADAPTIVE` and `hp_strategy` is `HP_REFSOLN_ELEM` or `HP_REFSOLN_EDGE`, the default is 21. If the element kind from running mkmkfile.sh is tetrahedron then the default is 10. If the element kind from running mkmkfile.sh is tetrahedron_fixdeg then if degree is present, then the default is degree, and if degree is not present, then the default is the maximum degree in the current grid.

`logical stop_on_maxlev` – if `.true.`, then max_lev is used as one of the termination criteria.

The default is `.false.`

`logical stop_on_maxdeg` – if `.true.`, then max_deg is used as one of the termination criteria.

The default is `.false.`

`integer max_refsolveloop` – number of times to go through the refine/solve loop (termination criteria).

The default is ∞, defined to be `huge(0)`.

`real(my_real) min_elem_size` – minimum element size; an element whose size is less than `min_elem_size` is treated the same as an element whose level is greater than or equal to `max_lev`. In 2D the size of an element is the square root of the area of the triangle. In 3D the size of an element is the cube root of the volume of the tetrahedron.

The default is 0.0.

`real(my_real) term_energy_err` – terminate when the energy error estimate is less than this value (termination criteria).

The default is 0.0.

`real(my_real) term_Linf_err` – terminate when the L^∞ error estimate is less than this value (termination criteria).

The default is 0.0.

`real(my_real) term_L2_err` – terminate when the L^2 error estimate is less than this value (termination criteria).

The default is 0.0.

`real(my_real) term_H1_err` – terminate when the H^1 error estimate is less than this value (termination criteria). Cannot be used with the hierarchical coefficient and explicit error estimators.

The default is 0.0.

`real(my_real) term_H1_seminorm_err` – terminate when the H^1 semi-norm error estimate is less than this value (termination criteria). Cannot be used with the hierarchical coefficient and explicit error estimators.

The default is 0.0.

`real(my_real) term_eigenvlaue_err` – terminate when the eigenvalue error estimate is less than this value (termination criteria).

The default is 0.0.

6.4.15.3 Output control arguments

`integer print_grid_when` – how often to produce a printed summary of the grid (number of vertices and elements, etc.). Valid values are:

`NEVER` – don't print.

`PHASES` – after each refinement phase.

`FINAL` – only at the end.

`FREQUENTLY` – possibly more often than `PHASES` (used for debugging).

The default is `NEVER`.

`integer print_grid_who` – which processes should print the summary of the grid. Valid values are:

NO_ONE – don't print.

SLAVES – slave processes print a summary of the grid as they know it.

MASTER – master process prints the composite grid.

EVERYONE – both SLAVES and MASTER.

MASTER_ALL – master prints the individual grids of each slave process.

The default is NO_ONE.

integer print_linsys_when – how often to produce a printed summary of the linear system (number of equations, sparsity, etc.). Valid values are:

NEVER – don't print.

PHASES – after each linear system assembly.

FREQUENTLY – possibly more often than PHASES (used for debugging).

The default is NEVER.

integer print_linsys_who – which processes should print the summary of the linear system. Valid values are:

NO_ONE – don't print.

SLAVES – slave processes print a summary of the system as they know it.

MASTER – master process prints the composite linear system.

EVERYONE – both SLAVES and MASTER.

MASTER_ALL – master prints the individual systems of each slave process.

The default is NO_ONE.

integer print_solver_when – how often to produce a printed summary of the solver performance (number of iterations, residual, etc.). Valid values are:

NEVER – don't print.

PHASES – after each linear system solution phase.

FREQUENTLY – possibly more often than PHASES (used for debugging).

The default is NEVER.

integer print_solver_who – which processes should print the summary of the solver performance. Valid values are:

NO_ONE – don't print.

SLAVES – slave processes.

MASTER – master process.

EVERYONE – both SLAVES and MASTER.

MASTER_ALL – master process.

The default is NO_ONE.

integer print_error_when – how often to print the norms of the error (defined to be the difference between the computed solution and the function defined in function true) and error estimates. It also prints the factor by which they have been reduced since the last time they were printed, and the effectivity index of the error estimate (ratio of the error estimate to the error) if both the error and error estimate are printed. If trues returns huge(0.0_my_real) to indicate that the true solution is not known, then the error is not printed. If truexs or trueys return huge(0.0_my_real) and trues does not, then the energy norm, H^1 norm, and H^1 semi-norm of the error (if requested) is printed as huge(0.0_my_real). Valid values are:

NEVER – don't print.

PHASES – after each solution phase.

FINAL – only at the end.

FREQUENTLY – possibly more often than PHASES (used for debugging). With the hierarchical basis multigrid solver, built in conjugate gradient and GMRES solvers, and the PETSc solvers, this causes an estimate of the ℓ^2 norm of the residual to be printed after each iteration. See KSPDefaultMonitor in the PETSc documentation. For GMRES_SOLVER it is only printed at the restarts.

TOO_MUCH – possibly more often than FREQUENTLY. Also this sets the solution to 0.0 before the solution phase as well as printing the residual after each iteration of some solvers as with FREQUENTLY.

The default is NEVER.

integer print_error_who – which processes should print the error. Individual processor energy norms of the error cannot be computed, so the energy norm of the error is printed only by the master. Valid values are:

NO_ONE – don't print.

SLAVES – slave processes print the error over the grid as they know it.

MASTER – master process prints the error over the composite grid.

EVERYONE – both SLAVES and MASTER.

MASTER_ALL – master prints the individual errors of each slave process.

The default is NO_ONE.

logical print_energy_norm_error – if .true. and norms of the error are printed, include the energy norm.

The default is .false.

`logical print_H1_norm_error` – if `.true.` and norms of the error are printed, include the H^1 norm.

The default is `.false.`

`logical print_H1_seminorm_error` – if `.true.` and norms of the error are printed, include the H^1 semi-norm.

The default is `.false.`

`logical print_Linf_norm_error` – if `.true.` and norms of the error are printed, include the L^∞ norm.

The default is `.false.`

`logical print_L2_norm_error` – if `.true.` and norms of the error are printed, include the L^2 norm.

The default is `.false.`

`logical print_energy_norm_errest` – if `.true.` and error estimates are printed, include the energy norm.

The default is `.false.`

`logical print_H1_norm_errest` – if `.true.` and error estimates are printed, include the H^1 norm. Cannot be used with the hierarchical coefficient and explicit error estimators.

The default is `.false.`

`logical print_H1_seminorm_errest` – if `.true.` and error estimates are printed, include the H^1 semi-norm. Cannot be used with the hierarchical coefficient and explicit error estimators.

The default is `.false.`

`logical print_Linf_norm_errest` – if `.true.` and error estimates are printed, include the L^∞ norm.

The default is `.false.`

`logical print_L2_norm_errest` – if `.true.` and error estimates are printed, include the L^2 norm.

The default is `.false.`

`integer errtype` – type of error and error estimates to use in printed output. Valid values are:

`ABSOLUTE_ERROR` – absolute error.

`RELATIVE_ERROR` – relative error. Norms of the error are scaled by the norm of the true solution. Error estimates are scaled by the norm of the computed solution.

The default is `ABSOLUTE_ERROR`.

`integer print_time_when` – how often to print the amount of time used by the program. Valid values are:

`NEVER` – don't print.

`PHASES` – after each refinement/solve loop.

`LAST` – the time for the last cycle.

`FINAL` – only at the end.

`LAST_AND_FINAL` – the time of the last cycle, and the total time.

`FREQUENTLY` – possibly more often than `PHASES` (used for debugging).

The default is `NEVER`.

`integer print_time_who` – which processes should print the time. Valid values are:

`NO_ONE` – don't print.

`SLAVES` – slave processes print their own times.

`MASTER` – master process prints maximum time over all slaves.

`EVERYONE` – both `SLAVES` and `MASTER`.

`MASTER_ALL` – master prints the individual times of each slave process.

The default is `NO_ONE`.

`integer clocks` – which clock(s) (cpu and/or wall) to use for timing. Valid values are:

`CLOCK_C` – cpu clock.

`CLOCK_W` – wall clock.

`CLOCK_CW` – both cpu and wall clock.

The default is `CLOCK_W`.

`integer print_eval_when` – for eigenvalue problems, how often to print the eigenvalues. Valid values are:

`NEVER` – don't print.

`PHASES` – after each refinement/solve loop.

`FINAL` – only at the end.

The default is `NEVER`.

`integer print_eval_who` – for eigenvalue problems, which processes should print the eigenvalues. Valid values are:

`NO_ONE` – don't print.

`SLAVES` – slaves print the eigenvalues.

MASTER – master process prints the eigenvalues.

EVERYONE – both SLAVES and MASTER.

The default is NO_ONE.

`integer print_header_who` – which processes should print a header message and the values of the parameters when the subroutine starts. Valid values are:

NO_ONE – don't print.

SLAVES – slaves print the header.

MASTER – master prints the header.

EVERYONE – both SLAVES and MASTER.

The default is MASTER.

`integer print_trailer_who` – which processes should print a trailer message when the subroutine completes. Valid values are:

NO_ONE – don't print.

SLAVES – slaves print the trailer.

MASTER – master prints the trailer.

EVERYONE – both SLAVES and MASTER.

The default is MASTER.

`logical print_warnings` – if `.false.`, warning messages are not printed.

The default is `.true.`

`integer draw_grid_when` – how often to update the graphics. Valid values are:

NEVER – don't draw.

PHASES – after each refinement and solve phase.

FINAL – only at the end.

FREQUENTLY – possibly more often than PHASES (used for debugging).

The default is NEVER.

`logical pause_after_draw` – if `.true.`, the program will prompt for keyboard input after updating the graphics.

The default is `.false.`

`logical pause_after_phases` – if `.true.`, the program will prompt for keyboard input after each refinement/solve loop.

The default is `.false.`

`logical pause_at_start` – if `.true.`, the program will prompt for keyboard input before starting subroutine `phaml_solve_pde`.

The default is `.false.`

`logical pause_at_end` – if `.true.`, the program will prompt for keyboard input before returning from subroutine `phaml_solve_pde`.

The default is `.false.`

6.4.15.4 Refinement arguments

`integer degree` – sets the initial degree of the polynomials in the finite element space. If no *p* refinement is performed, it is the fixed degree of the space.

In most cases the default is to use the existing degree in each element. In `phaml_create`, all elements are initialized to have degree 1. If the element kind from running mkmkfile.sh is tetrahedron_fixdeg and max_deg is present, then the default is max_deg.

`logical derefine` – if `.true.`, perform derefinement as well as refinement during adaptive refinement.

The default is `.true.`

`integer error_estimator` – select what to use for an error estimate to guide adaptive refinement and estimate global norms of the error. Valid values are:

`EXPLICIT_ERRIND` – error indicator based on the norm of the residual and jump.

`LOCAL_PROBLEM_H` – computes an estimate over a pair of elements by performing one *h* refinement and solving a local Diriclet residual problem.

`LOCAL_PROBLEM_P` – computes an estimate over a triangle by performing one *p* refinement and solving a local Neumann residual problem.

`EQUILIBRATED_RESIDUAL` – computes an estimate over a triangle by performing one *p* refinement and solving a local Neumann residual problem with an equilibrated residual.

`HIERARCHICAL_COEFFICIENT` – use the coefficient of the h-hierarchical basis for linear elements, or the highest order p-hierarchical bases for high order elements. It is significantly faster than the local problem estimates, but of lower quality.

`TRUE_DIFF` – use the difference between the true solution at the newest vertex of the element and surrounding vertices of the parent element. Can only be used if the true solution is known and supplied, and only for *h* refinement of linear elements.

`INITIAL_CONDITION` – an error estimate based on interpolation of the function in subroutine `iconds` (Section 6.3.5). If `task` is `SET_INITIAL` then it must be `INITIAL_CONDITION`.

The default is `EXPLICIT_ERRIND`, but it is always set to `INITIAL_CONDITION` if `task` is `SET_INITIAL`.

`integer reftype` – type of refinement to perform. Valid values are:

`H_UNIFORM` – uniform h refinement.

`H_ADAPTIVE` – adaptive h refinement.

`P_UNIFORM` – uniform p refinement.

`P_ADAPTIVE` – adaptive p refinement.

`HP_ADAPTIVE` – adaptive h and p refinement.

The default is `H_ADAPTIVE`.

`integer refterm` – termination criteria for a refinement phase (`DOUBLE` or `HALVE` really mean to multiply or divide by `inc_factor`). Valid values are:

`DOUBLE_NVERT` – double the number of vertices.

`DOUBLE_NELEM` – double the number of elements.

`DOUBLE_NEQ` – double the number of equations.

`HALVE_ERREST` – reduce the maximum error indicator by half.

`KEEP_NVERT` – keep the same number of vertices or, if max_vert is present, try to make it close to max_vert.

`KEEP_NELEM` – keep the same number of elements or, if max_elem is present, try to make it close to max_elem.

`KEEP_NEQ` – keep the same number of equations or, if max_eq is present, try to make it close to max_eq.

`ONE_REF` – (with default parameters) refine all elements with an error indicator larger than `reftol`$/\sqrt{n}$ where n is the number of elements, but refine each element only once (just h or p, and don't refine children).

`ONE_REF_HALF_ERRIND` – (with default parameters) perform one refinement of all elements with an error indicator larger than half (or 1/`inc_factor`) of the maximum error indicator.

`MATCH_TOL` – repeat the coarsen-refine loop until the error indicator of all coarsenable elements is larger than the coarsen cutoff and the error indicator of all refinable elements is less than the refine cutoff.

The default is `DOUBLE_NEQ`

`real(my_real) inc_factor` – usually the factor by which to increase the size of the grid during one refinement phase. For *hp*-adaptive refinement with REFSOLN_EDGE or REFSOLN_ELEM, it is the factor by which the maximum error indicator is divided to get the error indicator cut-off that determines which elements are refined.

The default is usually 2.0. For *hp*-adaptive refinement with REFSOLN_EDGE or REFSOLN_ELEM it is 10.0.

`real(my_real) reftol` – tolerance for determining the refine cutoff. If `refterm` is `ONE_REF` then at least one of `reftol`, or `term_energy_err` must be given. In addition to positive real numbers, valid values are:

`MAX_ERRIND_OVER_FACTOR` – base the refine cutoff on the maximum error indicator.

The default is `term_energy_err` if `refterm` is `ONE_REF`, and `MAX_ERRIND_OVER_FACTOR` otherwise.

`real(my_real) reftol_factor` – factor by which to divide `reftol`.

The default is 1.0 if `reftol` is given as a number, otherwise 2.0 if `refterm` is `ONE_REF`, `inc_factor` if `refterm` is `ONE_REF_HALF_ERRIND`, and 4.0 otherwise.

`real(my_real) coarsentol` – tolerance for determining the coarsen cutoff. In addition to positive real numbers, valid values are:

`MAX_ERRIND_OVER_FACTOR` – base the coarsen cutoff on the maximum error indicator.

`REFCUTOFF_OVER_FACTOR` – base the coarsen cutoff on the refine cutoff.

`REFCUTOFF_TIMES_CONVERGENCE` – base the coarsen cutoff on the refine cutoff and the asymptotic convergence rate.

The default is `REFCUTOFF_OVER_FACTOR` if `reftol` is given as a number or `refterm` is `ONE_REF`, and MAX_ERRIND_OVER_FACTOR otherwise.

`real(my_real) coarsentol_factor` – factor by which to divide `coarsentol`.

The default is 1.0 if `coarsentol` is given as a number, and 100.0 otherwise.

`integer recoarsen_limit` – if `refterm` is `MATCH_TOL` then the ban on coarsening an element whose parent was rerefined after it's children were coarsened is carried over from the previous refinement phase after the `recoarsen_limit`th time through the refine-solve loop if the change in the number of elements in the previous refinement phase was less than `recoarsen_tol` times the number of elements in the grid.

The default is 3.

`real(my_real) recoarsen_tol` – see `recoarsen_limit`.

The default is 0.01.

`logical reftol_scale_energy` – whether or not to scale `reftol` by the square root of the number elements and, if `errtype` is `RELATIVE_ERROR`, the energy norm of the computed solution.

The default is `.true.` if `refterm` is `ONE_REF`, and `.false.` otherwise.

`integer refmaxloop` – maximum number of times through the coarsen-refine loop within a refinement phase.

The default is 10.

`integer hp_strategy` – select strategy for `reftype=HP_ADAPTIVE`. See Section 3.3.2. Valid values are:

`HP_APRIORI` – use h refinement around *a priori* known trouble spots, and p refinement elsewhere. The regularity, m, of the solution is given by the user in function subroutine `regularity` (Sect. 6.3.8). h refinement is used if the degree of the element is larger than m.

`HP_NEXT3P` – *hp* strategy in which the regularity is estimated using error estimators computed with spaces of degree $p+1$, $p+2$, and $p+3$.

`HP_PRIOR2P_E` – *hp* strategy in which the regularity is estimated using energy norm error estimators computed with spaces of degree $p-1$ and $p-2$.

`HP_PRIOR2P_H1` – *hp* strategy in which the regularity is estimated using H^1 error estimators computed with spaces of degree $p-1$ and $p-2$.

`HP_TYPEPARAM` – the type parameter strategy.

`HP_BIGGER_ERRIND` – compute both `LOCAL_PROBLEM_H` and `LOCAL_PROBLEM_P` error indicators and refine an element by h or p depending on which is bigger.

`HP_PATCH` – solve the residual problem on a patch of elements refined by each of several candidates.

`HP_COEF_DECAY` – strategy based on the decay rate of the p-hierarchical coefficients.

`HP_COEF_ROOT` – strategy that estimates the regularity using a root test with the p-hierarchical coefficients.

`HP_SMOOTH_PRED` – a strategy that compares the local *a posteriori* error estimate with a predicted error estimate under the assumption that the solution is smooth.

`HP_REFSOLN_ELEM` – a strategy that considers several possible refinements of an element and picks one that reduces the difference from a reference solution the most.

`HP_REFSOLN_EDGE` – a strategy that considers several possible refinements of an edge and picks one that reduces the difference from a reference solution the most, and refines elements to be consistent with the chosen edge refinement.

The default is `HP_COEF_DECAY`.

`real(my_real) tp_gamma` – the type parameter γ for `HP_TYPEPARAM`.

The default is 0.8 for 2D and 1.2 for 3D, but it is recommended that for problems where the solution has a singularity you use 0.15 for 2D and 0.6 for 3D.

`real(my_real) sp_gamma_h` – parameter γ_h for `SMOOTH_PRED`.

The default is 10.0 in 2D and 4.0 in 3D.

`real(my_real) sp_gamma_p` – parameter γ_p for `SMOOTH_PRED`.

The default is 0.4.

`real(my_real) pbias` – bias the HP_REFSOLN_ELEM or HP_BIGGER_ERRIND strategy toward p-refinement. Recommended values for 2D problems are 2.0 for singular or nearly singular solutions and 4.0 for smooth solutions or moderately strong features, and for 3D problems 1.0, although a smaller value like 0.3 may be better for strong features. 1.0 is no bias.

The default is 4.0 in 2D and 1.0 in 3D.

`real(my_real) hp_patch_mult, and integer hp_patch_add` – candidate refinements for the HP_PATCH strategy; see 3.3.2

The default is HP_PATCH_H_P_CANDIDATES.

`integer edge_rule` – the rule for determining how to assign the polynomial degree for edges. Valid values are:

- `MINIMUM_RULE` – use the minimum of the degrees of the triangles sharing the edge.
- `MAXIMUM_RULE` – use the maximum of the degrees of the triangles sharing the edge.

The default is MINIMUM_RULE.

`integer p_compatibility` – determines how to enforce p compatibility of the grid. Valid values are:

- `PCOMPAT_NONE` – no p compatibility, i.e. there is no limit on how large the difference between the degrees of neighboring elements can be.
- `PCOMPAT_INCREASE` – if the degrees of neighboring elements differ by more than `max_p_diff`, increase the smaller one to the larger degree minus `max_p_diff`.
- `PCOMPAT_DECREASE` – if the degrees of neighboring elements differ by more than `max_p_diff`, decrease the bigger one to the smaller degree plus `max_p_diff`.

The default is PCOMPAT_NONE.

`integer max_p_diff` – if `p_compatibility` is not `PCOMPAT_NONE`, this is the maximum difference allowed in the degrees of neighboring elements.

The default is 1.

6.4.15.5 Load balancing arguments

`integer sequential_vert` – number of vertices in the grid before it starts running in parallel.

The default is 100.

`integer prebalance` – what to balance when partitioning the grid before refinement. Valid values are:

`BALANCE_NONE` – do not partition the grid before refinement.

`BALANCE_ELEMENTS` – equal number of elements in each partition.

`BALANCE_VERTICES` – equal number of vertices in each partition.

`BALANCE_EQUATIONS` – equal number of equations in each partition.

The default is `BALANCE_ELEMENTS`.

`integer postbalance` – what to balance when partitioning the grid after refinement. Valid values are:

`BALANCE_NONE` – do not partition the grid after refinement.

`BALANCE_ELEMENTS` – equal number of elements in each partition.

`BALANCE_VERTICES` – equal number of vertices in each partition.

`BALANCE_EQUATIONS` – equal number of equations in each partition.

The default is `BALANCE_NONE`.

`integer partition_method` – what method to use for partitioning the grid. Valid values are:

`RTK` – the k-way refinement tree method implemented in PHAML.

`ZOLTAN_RCB` – recursive coordinate bisection, from Zoltan.

`ZOLTAN_OCT` – RPI's Octree method, from Zoltan.

`ZOLTAN_METIS` – the local diffusion method from ParMETIS via Zoltan.

`ZOLTAN_REFTREE` – the refinement tree method, from Zoltan.

`ZOLTAN_RIB` – recursive inertial bisection, from Zoltan.

`ZOLTAN_HSFC` – Hilbert space filling curve, from Zoltan.

`ZOLTAN_FILE` – give Zoltan method and parameters in a file.

The default is `RTK`.

`character(len=*) zoltan_param_file` – name of the file containing parameters for ZOLTAN_FILE. The default is `zoltan.params`.

6.4.15.6 Assembly arguments

`integer inc_quad_order` – increment the order of the quadrature rules by this amount.

The default is 0.

`logical ignore_quad_err` – if `.true.`, when setting up the linear system, ignore the quadrature errors in the large triangles outside the owned region. This is acceptable (and reduces computation and communication) when the PDE coefficients and right hand side are constant (for example, Laplace's equation), or when using a solver other than HBMG, but will reduce the convergence of the discretization error otherwise.

The default is `.false.` if the solver is HBMG and `.true.` otherwise.

6.4.15.7 Solver arguments

`integer solver` – what method to use as the solver. Valid values are:

`MG_SOLVER` – the hierarchical basis multigrid method implemented in PHAML.

`CG_SOLVER` – conjugate gradient sovler implemented in PHAML.

`GMRES_SOLVER` – GMRES solver implemented in PHAML.

`PETSC_RICHARDSON_SOLVER` – Richardson solver from PETSc.

`PETSC_CHEBYCHEV_SOLVER` – Chebychev solver from PETSc.

`PETSC_CG_SOLVER` – Conjugate Gradients from PETSc.

`PETSC_GMRES_SOLVER` – Generalized Minimal Residual (GMRES) from PETSc.

`PETSC_TCQMR_SOLVER` – Transpose-Free Quasi-Minimal Residual (QMR) from PETSc.

`PETSC_BCGS_SOLVER` – BiConjugate Gradients Stabilized (BiCGSTAB) from PETSc.

`PETSC_CGS_SOLVER` – Conjugate Gradient Squared from PETSc.

`PETSC_TFQMR_SOLVER` – Transpose-Free Quasi-Minimal Residual (QMR) from PETSc.

`PETSC_CR_SOLVER` – Conjugate Residual from PETSc.

`PETSC_LSQR_SOLVER` – Least Squares from PETSc.

`PETSC_BICG_SOLVER` – BiConjugate Gradients from PETSc.

`PETSC_MUMPS_GEN_SOLVER` – Nonsymmetric direct solver from MUMPS.

`PETSC_MUMPS_SPD_SOLVER` – Symmetric positive definite direct solver from MUMPS.

`PETSC_SUPERLU_SOLVER` – Direct solver from SuperLU.

`PETSC_HYPRE_BOOMERAMG_SOLVER` – BoomerAMG algebraic multigrid from *hypre*.

`LAPACK_INDEFINITE_SOLVER` – the indefinite solver from LAPACK. This is available for certain debugging and testing operations, and can only be used for very small problem sizes and only with one processor.

`LAPACK_SPD_SOLVER` – the LAPACK solver for symmetric positive definite band matrices. This is available for certain debugging and testing operations, and can only be used for very small problem sizes and only with one processor.

The default is `MG_SOLVER` in 2D and PETSC_CG_SOLVER in 3D.

`integer preconditioner` – what method to use as a preconditioner for the Krylov methods. Valid values are:

`NO_PRECONDITION` – no preconditioning.

`MG_PRECONDITION` – a hierarchical basis multigrid V-cycle preconditioner.

`PETSC_JACOBI_PRECONDITION` – Jacobi preconditioner from PETSc.

`PETSC_BJACOBI_PRECONDITION` – Block Jacobi preconditioner from PETSc.

`PETSC_SOR_PRECONDITION` – SOR (and SSOR) preconditioner from PETSc.

`PETSC_EISENSTAT_PRECONDITION` – SOR with Eisenstat trick from PETSc.

`PETSC_ICC_PRECONDITION` – Incomplete Cholesky preconditioner from PETSc.

`PETSC_ILU_PRECONDITION` – Incomplete LU preconditioner from PETSc.

`PETSC_ASM_PRECONDITION` – Additive Schwarz preconditioner from PETSc.

`PETSC_GAMG_PRECONDITION` – Algebraic multigrid preconditioner from PETSc.

`PETSC_TRILINOS_ML_PRECONDITION` – Algebraic multigrid preconditioner from the ML package from Trilinos.

`PETSC_HYPRE_BOOMERAMG_PRECONDITION` – BoomerAMG algebraic multigrid from *hypre*.

`PETSC_HYPRE_PARASAILS_PRECONDITION` – ParaSails preconditioner from *hypre*.

`PETSC_HYPRE_PILUT_PRECONDITION` – Pilut preconditioner from *hypre*.

Note: For `solver=CG_SOLVER` and `solver=GMRES_SOLVER`, the preconditioner must be one of `NO_PRECONDITION` or `MG_PRECONDITION`.

The default is:

`NO_PRECONDITION` – when not applicable

`PETSC_SOR_PRECONDITION` – in 3D

`MG_PRECONDITION` – otherwise

`integer mg_cycles` – number of multigrid V-cycles to use in one solution phase or as a preconditioner.

If HBMG is the solver, then the default is 1 if `mg_tol` is `MG_NO_TOL` and infinite otherwise. If HBMG is the preconditioner, then the default is 2.

`real(my_real) mg_tol` – perform multigrid cycles until the ℓ^2 norm of the scaled linear system residual is less than `mg_tol` (up to a maximum of `mg_cycles` cycles). In addition to positive real numbers, it can have the following values:

`MG_NO_TOL` – do not use the tolerance test for ending the multigrid cycles, use a fixed number of cycles given by `mg_cycles` instead.

`MG_ERREST_TOL` – reduce the residual to some fraction of the error estimate, currently 1/1000.

The default is `MG_ERREST_TOL` if HBMG is the solver, and `MG_NO_TOL` if HBMG is the preconditioner.

`integer mg_prerelax` – number of half red-black relaxation sweeps to make before coarse grid correction in the *h*-hierarchical linear bases.

The default is 1.

`integer mg_postrelax` – number of half red-black relaxation sweeps to make after coarse grid correction in the *h*-hierarchical linear bases.

The default is 2.

`integer mg_prerelax_ho` – number of relaxation sweeps to make on each level of the high order *p*-multigrid cycle before coarse grid correction.

The default is 1.

`integer mg_postrelax_ho` – number of relaxation sweeps to make on each level of the high order *p*-multigrid cycle after coarse grid correction.

The default is 1.

`integer mg_comm` – selects how much communication to do in the parallel hierarchical basis multigrid method. Permitted values are

`MGCOMM_FUDOP` – the full domain partition approach with two messages per cycle.

`MGCOMM_CONVENTIONAL` – conventional communication at each level.

`MGCOMM_NONE` – no communication. Should only be used as a preconditioner.

The default is `MGCOMM_FUDOP` if HBMG is the solver and `MGCOMM_NONE` if HBMG is the preconditioner.

`integer krylov_iter` – the maximum number of iterations to use with the native Krylov space solvers `CG_SOLVER` and `GMRES_SOLVER`.

The default is 100.

`integer krylov_restart` – the GMRES restart parameter for `GMRES_SOLVER`.

The default is 20.

`real(my_real) krylov_tol` – convergence tolerance on the ℓ^2 norm of the linear system residual for the native Krylov space solvers. In addition to positive real numbers, it can have the following values:

- `KRYLOV_ERREST_TOL` – reduce the residual to some fraction of the error estimate, currently 1/100.

The default is `KRYLOV_ERREST_TOL`.

`logical petsc_matrix_free` – if the solver is one of the PETSc methods and this parameter is `.true.`, memory is saved by using a matrix-free approach that does not copy the matrix to a PETSc data structure. If `.true.`, then you cannot use the PETSc preconditioners.

The default is `.false.`

The following parameters are passed to subroutines in PETSc. See the documentation for PETSc for explanations and default values.

`real(my_real)`	`petsc_richardson_damping_factor`
`real(my_real)`	`petsc_chebychev_emin`
`real(my_real)`	`petsc_chebychev_emax`
`integer`	`petsc_gmres_max_steps`
`real(my_real)`	`petsc_rtol`
`real(my_real)`	`petsc_atol`
`real(my_real)`	`petsc_dtol`
`integer`	`petsc_maxits`
`integer`	`petsc_ilu_levels`
`integer`	`petsc_icc_levels`
`real(my_real)`	`petsc_sor_omega`
`integer`	`petsc_sor_its`
`integer`	`petsc_sor_lits`
`logical`	`petsc_eisenstat_nodiagscaling`
`real(my_real)`	`petsc_eisenstat_omega`
`integer`	`petsc_asm_overlap`

The following parameters are passed to subroutines in *hypre*. See the documentation for *hypre* for explanations and default values.

`real(my_real)`	`hypre_BoomerAMG_tol`
`real(my_real)`	`hypre_BoomerAMG_trunc_factor`
`real(my_real)`	`hypre_BoomerAMG_strong_threshold`
`real(my_real)`	`hypre_BoomerAMG_max_row_sum`
`real(my_real)`	`hypre_BoomerAMG_relax_weight`
`real(my_real)`	`hypre_BoomerAMG_outer_relax_weight`
`integer`	`hypre_BoomerAMG_cycle_type`
`integer`	`hypre_BoomerAMG_max_levels`
`integer`	`hypre_BoomerAMG_max_iter`
`integer`	`hypre_BoomerAMG_P_max_elmts`
`integer`	`hypre_BoomerAMG_agg_num_levels`
`integer`	`hypre_BoomerAMG_agg_num_paths`
`integer`	`hypre_BoomerAMG_num_sweeps_all`
`integer`	`hypre_BoomerAMG_num_sweeps_down`
`integer`	`hypre_BoomerAMG_num_sweeps_up`
`integer`	`hypre_BoomerAMG_num_sweeps_coarsest`
`integer`	`hypre_BoomerAMG_relax_type_all`
`integer`	`hypre_BoomerAMG_relax_type_down`
`integer`	`hypre_BoomerAMG_relax_type_up`
`integer`	`hypre_BoomerAMG_relax_type_coarsest`
`integer`	`hypre_BoomerAMG_relax_order`
`integer`	`hypre_BoomerAMG_measure_type`
`integer`	`hypre_BoomerAMG_coarsen_type`
`integer`	`hypre_BoomerAMG_interp_type`
`logical`	`hypre_BoomerAMG_print_statistics`
`logical`	`hypre_BoomerAMG_print_debug`
`real(my_real)`	`hypre_Pilut_tol`
`integer`	`hypre_Pilut_maxiter`
`integer`	`hypre_Pilut_factorrowsize`
`real(my_real)`	`hypre_ParaSails_thresh`
`real(my_real)`	`hypre_ParaSails_filter`
`real(my_real)`	`hypre_ParaSails_loadbal`
`integer`	`hypre_ParaSails_nlevels`
`integer`	`hypre_ParaSails_sym`
`logical`	`hypre_ParaSails_logging`
`logical`	`hypre_ParaSails_reuse`

6.4.15.8 Eigenvalue arguments

`integer eigensolver` – What method to use to solve the discrete eigenproblem. Valid values are:

`SLEPC_POWER` – SLEPc power iteration

`SLEPC_SUBSPACE` – SLEPc subspace iteration

`SLEPC_ARNOLDI` – SLEPc Arnoldi method

`SLEPC_LANCZOS` – SLEPc Lanczos method

`SLEPC_KRYLOV_SCHUR` – SLEPc Krylov-Schur method

`SLEPC_GEN_DAVIDSON` – SLEPc generalized Davidson

`SLEPC_JACOBI_DAVIDSON` – SLEPc Jacobi-Davidson

`SLEPC_LAPACK` – SLEPc wrapper to LAPACK

`SLEPC_ARPACK` – SLEPc wrapper to ARPACK

`SLEPC_BLOPEX` – SLEPc wrapper to BLOPEX

The default is `SLEPC_KRYLOV_SCHUR`.

`integer num_eval` – The number of eigenvalues to find.

The default is 1.

`real(my_real) lambda0` – Find the eigenvalues closest to `lambda0`.

The default is `-huge(0.0_my_real)`, i.e., find the smallest eigenvalues.

`integer transformation` – What spectral transformation to use. Valid values are:

`ST_NONE` – no spectral transformation

`ST_SHIFT_ORIGIN` – shift of origin

`ST_SHIFT_INVERT` – shift and invert

`ST_CAYLEY` – generalized Cayley

The default is `ST_NONE`.

`real(my_real) st_shift` – the shift for the SLEPc spectral transformations

The default is `lambda0`.

`real(my_real) st_antishift` – the antishift for the ST_CAYLEY spectral transformations

The default is to be the same as st_shift.

`integer scale_evec` – The eigenvectors can be multiplied (scaled) by an arbitrary constant. These are the choices for scaling:

`SCALE_LINF` – scale so the (discrete) ℓ^∞ norm is 1. For linear elements, this is also the L^∞ norm.

`SCALE_L2` – scale so the (discrete) ℓ^2 norm is 1.

`SCALE_M` – scale so the M norm, $\sqrt{x^T M x}$, is 1, where M is the mass matrix. The M norm is also the (continuous) L^2 norm.

The default is `SCALE_LINF`.

`integer eigen_ncv` – The number of column vectors to use in the eigensolver

The default is given in the SLEPc user's guide.

`integer eigen_maxit` – The maximum number of iterations to use in the eigensolver

The default is given in the SLEPc user's guide.

`real(my_real) eigen_tol` – The tolerance on the residual of the eigensystem

The default is 10^{-10}.

`logical harmonic_extraction` – If true, use harmonic extraction to accelerate convergence of interior eigenvalues.

The default is `.false.`

`logical slepc_true_residual` – For Krylov solvers use the true residual instead of a cheap approximation.

The default is `.false.`

6.4.16 phaml_store

`phaml_store` stores information from `phaml_solution` into files for later use.

```
subroutine phaml_store(phaml_solution, unit)
```

`type (phaml_solution_type), intent(in) :: phaml_solution` – the solution to store.

`integer, intent(in) :: unit` – the unit number to write to, which should have been opened as either FORMATTED or UNFORMATTED with subroutine `phaml_popen`. UNFORMATTED is likely to be faster and create smaller data files. FORMATTED may be required if you will be restoring with a different compiler or architecture, and might not reproduce floating point numbers exactly.

6.4.17 phaml_store_grid

`phaml_store_grid` stores the grid, and optionally the solution, to data files.

```
subroutine phaml_store_grid(phaml_solution, unit, fmt, comp, eigen,
noboundary, notags, only_gmsh)
```

`type (phaml_solution_type), intent(in) :: phaml_solution` – the solution containing the grid to store.

`integer, intent(in) :: unit` – the I/O unit number to which to write the grid. It should be open for formatted sequential writing prior to calling `phaml_store_grid` and closed afterwards.

`integer, intent(in) ::` `fmt` – the format for the output file. Valid values are:

- `GRIDFILE_POLY` – for 2D, store just the grid in triangle's .poly format, `http://www.cs.cmu.edu/~quake/triangle.poly.html`
- `GRIDFILE_POLY_SOLN` – for 2D, store both the grid and the solution in triangle's .poly format.
- `GRIDFILE_MSH` – for 2D or 3D, store just the grid in Gmsh's .msh format, `http://geuz.org/gmsh/doc/texinfo/gmsh.html#MSH-ASCII-file-format`
- `GRIDFILE_MSH_SOLN` – for 2D or 3D, store both the grid and the solution in Gmsh's .msh format.

`integer, intent(in), optional ::` `comp` – for multicomponent solutions, which component to store. The default is all of them.

`integer, intent(in), optional ::` `eigen` – for eigenvalue problems, which eigenfunction to store. The default is all of them.

`logical, intent(in), optional ::` `noboundary` – if `.true.`, only the elements are saved, not the boundary entities. The default is `.false.`

`logical, intent(in), optional ::` `notags` – if `.true.`, tags are not saved, except for a tag containing `bmark` for boundary entities. The default is `.false.`

`logical, intent(in), optional ::` `only_gmsh` – in 3D msh format, if `.true.`, only the elements plus the vertices, edges and faces that were "elements" in the original geo or msh file, and their descendants, are saved. The default is `.false.`

6.4.18 phaml_store_matrix

`phaml_store_matrix` stores the stiffness matrix, right hand side, and/or mass matrix in a file in Matrix Market exchange format (`http://math.nist.gov/MatrixMarket/formats.html`). For details, see Section 3.6.2.

```
   subroutine phaml_store_matrix(phaml_solution, stiffness_unit, rhs_unit,
mass_unit, inc_quad_order)
```

`type (phaml_solution_type), intent(in) ::` `phaml_solution` – the solution containing the linear system to store.

`integer, intent(in), optional ::` `stiffness_unit, rhs_unit, mass_unit` – the I/O unit numbers for writing the stiffness matrix, right hand side, and mass matrix, respectively. They should be open for formatted sequential writing prior to calling phaml_store_matrix and closed afterwards. Which ones are present determines which are written.

`integer, intent(in), optional ::` `inc_quad_order` – increase the order of the quadrature rule by this amount. Default is 0.

Bibliography

[1] M. Ainsworth and J.T. Oden, A Posteriori Error Analysis in Finite Element Analysis, Wiley Interscience Publishers, New York, 2000.

[2] M. Ainsworth and B. Senior, *hp*-finite element procedures on non-uniform geometric meshes: adaptivity and constrained approximation, in Grid Generation and Adaptive Algorithms, M. W. Bern and J. E. Flaherty and M. Luskin, eds, Vol. 113, IMA Volumes in Mathematics and its Applications, Springer-Verlag, New York, (1999), pp. 1-28.

[3] P.R. Amestoy, I.S. Duff, J. Koster and J.-Y. L'Excellent, A fully asynchronous multifrontal solver using distributed dynamic scheduling, SIAM Journal of Matrix Analysis and Applications, **23**, (1), (2001), pp. 15–41.

[4] P.R. Amestoy, A. Guermouche, J.-Y. L'Excellent and S. Pralet, Hybrid scheduling for the parallel solution of linear systems, Parallel Computing **32** (2), (2006), pp. 136–156.

[5] E. Anderson, Z. Bai, C. Bischof, J. Demmel, J. Dongarra, J. Du Croz, A. Greenbaum, S. Hammarling, A. McKenney, and D. Sorensen, LAPACK User's Guide, Third Edition, SIAM, Philadelphia, PA, USA, 1999.

[6] D. Arnold, A. Mukherjee and L. Pouly, Locally Adapted Tetrahedral Meshes Using Bisection, SIAM Journal on Scientific Computing **22** (2), (2000), pp. 431–448.

[7] S. Balay, V. Eijkhout, W.D. Gropp, L. Curfman!McInnes and B.F. Smith, Efficient Management of Parallelism in Object Oriented Numerical Software Libraries, in Modern Software Tools in Scientific Computing, E. Arge, A. M. Bruaset and H. P. Langtangen, eds., pp. 163–202, Birkhäuser Press, 1997.

[8] S. Balay, K. Buschelman, V. Eijkhout, W.D. Gropp, D. Kaushik, M.G. Knepley, L. Curfman McInnes, B.F. Smith and H. Zhang, PETSc Users Manual, ANL-95/11 - Revision 2.1.5, Argonne National Laboratory, 2004.

[9] R. Barrett, M. Berry, T. F. Chan, J. Demmel, J. Donato, J. Dongarra, V. Eijkhout, R. Pozo, C. Romine and H. Van der Vorst, Templates for the

Solution of Linear Systems: Building Blocks for Iterative Methods, Second Edition, SIAM, Philadelphia, PA, 1994.

[10] M. Bürg and W. Dörfler, Convergence of an Adaptive *hp* Finite Element Strategy in Higher Space-dimensions, Appl. Numer. Math., **61**, (2011), pp. 1132–1146.

[11] C. Campos, J.E. Román, E. Romero and A. Tomás, SLEPc Users Manual, available at `http://www.grycap.upv.es/slepc`

[12] P. Carnevali, R.B. Morris, Y. Tsuji and G. Taylor, New Basis Functions and Computational Procedures for the p-Version Finite Element Analysis, Int. J. Num. Meth. Engng., **36**, (1993), pp. 3759–3779.

[13] L. Demkowicz, Computing with hp-Adaptive Finite Elements, Volume 1, One and Two Dimensional Elliptic and Maxwell Problems, Chapman & Hall/CRC, Boca Raton, FL, 2007.

[14] K. Devine, B. Hendrickson, E. Boman, M. St. John, C. Vaughan and W.F. Mitchell, Zoltan: A dynamic load-balancing library for parallel applications, User's Guide, Sandia Technical Report SAND99-1377, Sandia National Laboratories, Albuquerque, NM, 2000.

[15] K. Devine, E. Boman, R. Heaphy, B. Hendrickson, C. Vaughan, Zoltan Data Management Services for Parallel Dynamic Applications, Computing in Science and Engineering, **4**, (2), (2002), pp. 90–97.

[16] R.D. Falgout and U.M. Yang, hypre: a Library of High Performance Preconditioners, in Computational Science - ICCS 2002 Part III, P.M.A. Sloot, C.J.K. Tan. J.J. Dongarra, and A.G. Hoekstra, eds., vol. 2331 of Lecture Notes in Computer Science, Springer-Verlag, 2002, pp. 632–641.

[17] R.D. Falgout, J.E. Jones, and U.M. Yang, The Design and Implementation of hypre, a Library of Parallel High Performance Preconditioners, in Numerical Solution of Partial Differential Equations on Parallel Computers, A.M. Bruaset, P. Bjrstad, and A. Tveito, eds., Lecture Notes in Computational Science and Engineering, Springer-Verlag, **51**, (2006), pp. 267–294.

[18] J. Faik, A Model for Resource-Aware Load Balancing on Heterogeneous and Non-Dedicated Clusters, PhD Thesis, Rensselaer Polytechnic Institute, Troy, NY, 2005.

[19] C. Geuzaine and J.-F. Remacle, Gmsh: a three-dimensional finite element mesh generator with built-in pre- and post-processing facilities, Int. J. Num. Meth. Eng., **79**, 11, (2009), pp. 1309–1331.

[20] C. Geuzaine and J.-F. Remacle, Gmsh web page, `http://geuz.org/gmsh/`

[21] W. Gui and I. Babuška, The *h*, *p* and *h-p* Versions of the Finite Element Method in 1 Dimension. Part 3: The Adaptive *h-p* Version, Numer. Math., **49**, (1986), pp. 659–683.

[22] P. Houston, B. Senior and E. Süli, Sobolev Regularity Estimation for *hp*-Adaptive Finite Element Methods, Numerical Mathematics and Advanced Applications (Berlin) (F. Brezzi, A. Buffa, S. Corsaro and A. Murli, eds.), Springer-Verlag, 2003, pp. 619–644.

[23] A. Knyazev, Toward the Optimal Preconditioned Eigensolver: Locally Optimal Block Preconditioned Conjugate Gradient Method, SIAM J. Sci. Comp., **23**, (2001), pp. 517–541.

[24] A. Knyazev, BLOPEX web page, `http://www-math.cudenver.edu/~aknyazev/software/BLOPEX/`

[25] R.B. Lehoucq, D.C. Sorensen, and C. Yang, ARPACK Users' Guide: Solution of Large-Scale Eigenvalue Problems with Implicitly Restarted Arnoldi Methods, SIAM, Philadelphia, 1998.

[26] X.S. Li and J.W. Demmel, SuperLU_DIST: A Scalable Distributed-Memory Sparse Direct Solver for Unsymmetric Linear Systems, ACM Trans. Math. Soft., **29**, (2), (2003), pp. 110–140.

[27] C. Mavriplis, Adaptive Mesh Strategies for the Spectral Element Method, Comput. Methods Appl. Mech. Engrg., **116**, (1994), pp. 77–86.

[28] J.M. Melenk and B.I. Wohlmuth, On Residual-based a-posteriori Error Estimation in *hp*-FEM, Adv. Comput. Math. **15** (2001), pp. 311–331.

[29] W.F. Mitchell, Adaptive refinement for arbitrary finite element spaces with hierarchical bases, J. Comp. Appl. Math., **36**, (1991), pp. 65–78.

[30] W.F. Mitchell, Optimal multilevel iterative methods for adaptive grids, SIAM J. Sci. Statist. Comput., **13**, (1992), pp. 146–167.

[31] W.F. Mitchell, The Full Domain Partition Approach to Parallel Adaptive Refinement, in Grid Generation and Adaptive Algorithms, IMA Volumes in Mathematics and its Applications, **113**, Springer-Verlag, 1998, pp. 151–162.

[32] W.F. Mitchell, A Parallel Multigrid Method Using the Full Domain Partition, Electronic Transactions on Numerical Analysis, **6**, (1998), pp. 224–233.

[33] W.F. Mitchell, A Refinement-tree Based Partitioning Method for Dynamic Load Balancing with Adaptively Refined Grids, J. Par. Dist. Comput., **67** (4), (2007), pp. 417–429.

[34] W.F. Mitchell, The *hp*-Multigrid Method Applied to *hp*-Adaptive Refinement of Triangular Grids, Num. Lin. Alg. Appl., **17** (2010), pp. 211–228.

[35] W.F. Mitchell and M.A. McClain, A Survery of *hp*-Adaptive Strategies for Elliptic Partial Differential Equations,Annals of the European Academy of Sciences, in Recent Advances in Computational and Applied Mathematics (T.E. Simos, ed.), Springer, 2011, pp. 227–258.

[36] W.F. Mitchell and M.A. McClain, A Comparison of *hp*-Adaptive Strategies for Elliptic Partial Differential Equations (long version), NISTIR 7824, 2011.

[37] W.F. Mitchell and M.A. McClain, A Comparison of *hp*-Adaptive Strategies for Elliptic Partial Differential Equations, submitted. Available at `http://math.nist.gov/~WMitchell`

[38] J.T. Oden and A. Patra, A parallel adaptive strategy for *hp* finite element computations, Comput. Methods Appl. Mech. Engrg., **121**, (1995), pp. 449–470.

[39] A. Patra and A. Gupta, A systematic strategy for simultaneous adaptive *hp* finite element mesh modification using nonlinear programming, Comput. Methods Appl. Mech. Engrg., **190**, (2001), pp. 3797–3818.

[40] J.R. Rice, Algorithm 625: A Two Dimensional Domain Processor, ACM Trans. Math. Soft., **10**, (1984), pp. 443–452.

[41] A. Schmidt and K.G. Siebert, a Posteriori Estimators for the $h-p$ Version of the Finite Element Method in 1D, Appl. Numer. Math., **35**, (2000), pp. 43–66.

[42] J.R. Shewchuk, Triangle: Engineering a 2D Quality Mesh Generator and Delaunay Triangulator, in Applied Computational Geometry: Towards Geometric Engineering (Ming C. Lin and Dinesh Manocha, editors), volume 1148 of Lecture Notes in Computer Science, pp. 203–222, Springer-Verlag, Berlin, May 1996.

[43] J.R. Shewchuk, Triangle: A Two-Dimensional Quality Mesh Generator and Delaunay Triangulator, `http://www.cs.cmu.edu/~quake/triangle.html`

[44] P. Šolín, J. Červený and I. Doležel, Arbitrary-level hanging nodes and automatic adaptivity in the *hp*-FEM, Math. Comput. Simulation **77** (2008), 117–132.

[45] G. Strang and G. Fix, An Analysis of the Finite Element Method, Prentice-Hall, Englewood Cliffs, NJ, 1973.

[46] E. Süli, P. Houston and Ch. Schwab, *hp*-Finite Element Methods for Hyperbolic Problems, in The Mathematics of Finite Elements and Applications X. MAFELAP, J.R. Whiteman (ed.), Elsevier, 2000, 143–162.

[47] B. Szabo and I. Babuška, Finite Element Analysis, John Wiley and Sons, New York, 1991.

[48] J.D. Teresco, J. Faik, and J.E. Flaherty, Resource-Aware Scientific Computation on a Heterogeneous Cluster, Computing in Science & Engineering, **7** (2), (2005), 40–50.

[49] J.D. Teresco, zoltanParams: Library for Parsing Zoltan Parameters, `http://www.cs.williams.edu/~terescoj/research/zoltanParams/`

[50] Trilinos web page, `http://trilinos.sandia.gov/`

[51] E.L. Wilson, The static condensation algorithm, Int. J. Num. Meth. Engrg., **8**, (1974), pp. 198–203.