

ScalES-PPM - Feature # 347

Status:	New	Priority:	Normal
Author:	Matthew Krupcale	Category:	
Created:	09/26/2017	Assignee:	
Updated:	09/26/2017	Due date:	

Subject: Add support for METIS v4-5 and ParMETIS v3-4

Description

Introduction

The current ScalES-PPM API appears to be designed around the METIS v4 and ParMETIS v3 APIs. The attached patch aims to add support for both METIS v4 and v5 as well as ParMETIS v3 and v4.

Summary of the patched files

- `configure.ac`: detect METIS and ParMETIS version; check `idx_t/idx_t` compatibility; check `real_t` compatibility
- `include/f77/ppm.inc.in`: define parameter `PPM_REAL` to be the width of `real_t`
- `ppm.settings.in`: define `ParMETIS/METIS fcrealkind` to be the width of `real_t`
- `src/Makefile.am`: define `HAVE_METIS_V4` and `HAVE_PARMETIS_V3` compiler preprocessor macros as needed; only in ParMETIS v3 include `src/ppm/parmetis_wrap.c` in `libscalesppm`
- `src/ppm/ppm_graph_partition_mpi.f90`: adjust INTERFACE SUBROUTINE `parmetis_v3_partkway` C-binding for particular version of ParMETIS; use `c_null_ptr` instead of all combinations of `dummy_{balance,weights}`
- `ppm_graph_partition_serial.f90`: define INTERFACE SUBROUTINE `metis_mcpartgraphkway`, INTERFACE SUBROUTINE `metis_setdefaultoptions`, and INTERFACE SUBROUTINE `metis_partgraphkway` C-bindings for particular version of METIS; use `c_null_ptr` instead of all combinations of `{v,e}w_dummy`

Detailed changes

`configure.ac`

There have been several changes made between METIS v4 and v5 in particular, making `configure.ac` and `ppm/ppm_graph_partition_serial.f90` inoperable with METIS v5. Some of the particular changes between METIS v4 and v5 are:

- Changed `idx_t` -> `idx_t`
- Unified routines (`METIS_PartGraphKway`, `METIS_mCPartGraphKway`, `METIS_WPartGraphKway`, `METIS_PartGraphVKway`, `METIS_WPartGraphVKway`) -> `METIS_PartGraphKway` (with a change in API)

ParMETIS v4 now also directly relies on METIS v5 and thus should not in principle have a different `idx_t` than METIS, unless the user explicitly builds METIS with `IDXTYPEWIDTH 32` and `IDXTYPEWIDTH 64`, then builds a modified version of ParMETIS v4. This would have to be a modified ParMETIS v4 because it directly includes the `metis.h`, where `idx_t` is typedef'd. Obviously this is not a supported configuration, and I would hope that the user would not attempt this. Nevertheless, if the user does this, the patched `configure.ac` still checks both `parmetis.h` and `metis.h` for the `idx_t/idx_t` and ensures that they are compatible.

Similarly to `idx_t`, METIS v5 now defines `real_t` rather than `float` for some of the balancing constraints. Thus, the patched `configure.ac` also checks for `real_t` (again in both `parmetis.h` and `metis.h`, in case the user tries to do something strange) and makes sure they are compatible. Note that this relies on the patch in #343.

These are the major changes to `configure.ac`. In addition to the above changes, `METIS_HEADER='metis/memis.h'` was removed because I could find no reference to such a file in any of the METIS installations and assumed this must be some custom installation location. In this case, the `metis.h` header location should be specified in the `configureCFLAGS` instead. If desired I can break this change out into a separate bug/patch, but it was causing issues when configuring my METIS/ParMETIS setups.

`src/Makefile.am`

A Fortran to C wrapper for `ParMETIS_V3_PartKway` is included in `src/ppm/parmetis_wrap.c` since the ParMETIS v3 Fortran wrapper does not include the conversion from Fortran MPI communicator to C MPI communicator, while the v4 API does this properly (see macro `FRENAME` in `parmetis-4.0.3/libparmetis/frename.c`), so this wrapper is only included in `libscalesppm` when using ParMETIS v3.

`src/ppm/ppm_graph_partition_mpi.f90`

ParMETIS_V3_PartKway function has the following prototypes in v 3.2.0 and v 4.0.3, respectively:

```
// ParMETIS v 3.2.0
void __cdecl ParMETIS_V3_PartKway(
    idxtype *vtxdist, idxtype *xadj, idxtype *adjncy, idxtype *vwgt,
    idxtype *adjwgt, int *wgflag, int *numflag, int *ncon, int *nparts,
    float *tpwgts, float *ubvec, int *options, int *edgecut, idxtype *part,
    MPI_Comm *comm);

// ParMETIS v 4.0.3
int __cdecl ParMETIS_V3_PartKway(
    idx_t *vtxdist, idx_t *xadj, idx_t *adjncy, idx_t *vwgt,
    idx_t *adjwgt, idx_t *wgflag, idx_t *numflag, idx_t *ncon, idx_t *nparts,
    real_t *tpwgts, real_t *ubvec, idx_t *options, idx_t *edgecut, idx_t *part,
    MPI_Comm *comm);
```

Thus, the types defined in the INTERFACE SUBROUTINE `parmetis_v3_partkway` had to be adjusted depending on the version of the library used.

The method for invoking `parmetis_v3_partkway` was also modified to require only one CALL site with the arguments passed depending on the presence of the OPTIONAL arguments to `graph_partition_parmetis`. In particular, several `TYPE(c_ptr)` were used and passed (by value) to the `parmetis_v3_partkway` Fortran C-binding rather than using an uninitialized dummy array. This scales much better with the number of optional arguments: for N optional arguments, there are 2^N combinations, while defining a pointer to either NULL or the location of the argument when present scales linearly in N .

Although `balance` is an OPTIONAL argument, `tpwgts` appears to be required in the ParMETIS v4 API (see `parmetis-4.0.3/libparmetis/weird.c:CheckInputsPartKway`), and thus `balance` is constructed with equal weights for each sub-domain/partition when it is not present.

ppm_graph_partition_serial.f90

METIS v4 has separate routines for multi-constraint partitioning (`METIS_mCPartGraphKway`) and single-constraint partitioning (`METIS_PartGraphKway`); in METIS v5, these two partitioning methods are unified into `METIS_PartGraphKway` (albeit with different API than in v4). METIS v5 also has a larger set of options and a corresponding function `METIS_SetDefaultOptions` to initialize it with defaults. Only `METIS_OPTION_NUMBERING` is set (corresponding to `numflag` in the v4 API) to indicate Fortran-style numbering.

The `METIS_PartGraphKway` function has the following prototypes in v 4.0.3 and v 5.1.1, respectively:

```
// METIS v 4.0.3
void METIS_PartGraphKway(int *nvtxs, idxtype *xadj, idxtype *adjncy, idxtype *vwgt,
    idxtype *adjwgt, int *wgflag, int *numflag, int *nparts,
    int *options, int *edgecut, idxtype *part);

// METIS v 5.1.0
METIS_API(int) METIS_PartGraphKway(idx_t *nvtxs, idx_t *ncon, idx_t *xadj,
    idx_t *adjncy, idx_t *vwgt, idx_t *vsize, idx_t *adjwgt,
    idx_t *nparts, real_t *tpwgts, real_t *ubvec, idx_t *options,
    idx_t *edgecut, idx_t *part);
```

Thus, similar to in `src/ppm/ppm_graph_partition_mpi.f90`, the types and parameters defined in the INTERFACE SUBROUTINE `metis_partgraphkway` had to be adjusted depending on the version of the library used. Additionally, like in `src/ppm/ppm_graph_partition_mpi.f90`, `c_null_ptr` was used to indicate the absence of OPTIONAL arguments, and a single CALL site was used for all combinations of OPTIONAL arguments.

Supported combinations of METIS and ParMETIS

While this patch is designed for use with arbitrary combinations of METIS v4/v5 and ParMETIS v3/v4, in practice, when using ParMETIS, I expect this to only work when building ParMETIS with the internally-bundled version of METIS or with ParMETIS v4.0.3 and an internal or external METIS v5.

By default, it is not possible to build binaries linked against ParMETIS v3+ and external METIS v4 package because the ParMETIS v3 version of parmetis.c (modified from the METIS version) defines functions METIS_NodeRefine (needed by ParMETIS v3.2+) and/or METIS_mCPartGraphRecursive2 (needed by ParMETIS v3). So in order to use an external METIS v4 with ParMETIS v3, the METIS v4 parmetis.c would have to be similarly modified to define these functions. However, it is possible to build binaries linked against ParMETIS v4 and external METIS v5 since it defines METIS_NodeRefine. This should also be clear from the fact that ParMETIS v4 now uses and bundles METIS v5 directly.

In spite of still technically supporting METIS v4 and ParMETIS v3, the only combination really recommended is METIS v5 and ParMETIS v4. In testing (using example/graph_partition), METIS v4 seems to be unreliable, returning SIGABRT double free or corrupted double-linked list or SIGSEGV segmentation fault errors within METIS_mCPartGraphKway. Thus, the multi-constraint procedure in METIS v4 seems altogether un-usable. These errors do not appear in the METIS v5 version. Both of these codes are more than 5 years old at this point, so I would hope that this is not much of an issue.

Testing

Since my goal is to package ScaLES-PPM for Fedora, I am working on this on Fedora, and I have some Bash scripts which setup a mock chroot, build METIS v4 and ParMETIS v3/4, and build ScaLES-PPM with various combinations of these. Let me know if you are interested in trying out these tests.

History

Files

scales-ppm-metis-4-5-parmetis-3-4.patch	22.7 kB	09/26/2017	Matthew Krupcale
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