FUN3D v13.4 Training
Session 3:
Compilation and Installation

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Learning Goals

- What this will teach you
  - How to configure and compile the FUN3D suite
  - Configuration options
    - Enable/Disable capabilities
    - Specify the location of 3rd party libraries and tools
  - How we do it
- What you will not learn
  - How to build/install 3rd party libraries and tools
  - How to configure your system to compile Fortran 90/MPI code
- What should you already know
  - How to navigate through a *NIX shell
    - **`mkdir`**
    - **`cd`**
    - Absolute/relative paths

Setting

- Background
  - FUN3D uses the de facto industry standard build environment provided by GNU Autotools
  - Build of the FUN3D distribution does **not** require Autotools on your system
  - Provides localization through options to a configuration script
- Compatibility
  - Requires a Bourne Shell derivative (*NIX, OS X, MinGW, etc.)
  - Requires GNU `**make**`
  - Requires a functioning Fortran 95 compliant compiler (some optional capabilities rely on Fortran 2003 additions)
  - May not work with non-standard installation of 3rd party libraries
  - DiRTLib and SUGGAR++ assumptions for overset support
  - Required library names: **`libp3d.a, libdirt.a, libdirt_mpich.a, libsuggar.a, and libsuggar_mpi.a`**
  - Developers will need GNU Autotools installed

Nuts and Bolts (1 of 4)

- Two step process
  - `**configure**` selects capabilities and localizes to system
  - `**make**` creates executables
- Distribution contains a `**configure**` script
  - Familiar to Linux users/administrators who have built open source packages
  - Must **NOT** be edited by hand
  - Custom localization through command line options
- The `**configure**` script creates **Makefiles**
  - **Makefiles** are customized/localized for a specific configuration
  - Not practical for human consumption
  - Must **NOT** be edited by hand
  - All localization is managed through the `**configure**` script
  - Checks various details required by compilation
  - Fails fast (prior to compilation of FUN3D) if problems are detected with the configuration options (no compiler, missing libraries, etc.)

Nuts and Bolts (2 of 4)

- **`configure --help`** will show a list of all options
  - Command line options
  - Environment variables
  - Order independent (uses last value if specified multiple times)
- FUN3D optional Features of general interest

`--disable-FEATURE` do not include FEATURE
(same as **`--enable-FEATURE=no`**)

`--enable-FEATURE[=ARG]` include FEATURE **`[ARG=yes]`**

`--enable-hefss` build with High Energy Physics **`[no]`**

`--enable-ftune` tailor Fortran compiler options for FUN3D **`[yes]`**

Nuts and Bolts (3 of 4)

- FUN3D optional Packages of general interest

--with-PACKAGE[=ARG] use PACKAGE [ARG=yes]
--without-PACKAGE do not use PACKAGE (same as **--with-PACKAGE=no**)

--with-mpi[=ARG] Path to MPI library (installation root)
--with-mpif90[=ARG] MPI Fortran compiler wrapper (relative, absolute, without)
--with-mpicc[=ARG] MPI C compiler wrapper (relative, absolute, without)
--with-mpicxx[=ARG] MPI C++ compiler wrapper (relative, absolute, without)
--with-mpiexec[=ARG] MPI execution startup script (relative, absolute, without)
--with-mpibin[=ARG] MPI binary directory (relative, absolute, without)
--with-mpiinc[=ARG] Path to "mpif.h" (relative, absolute, without)
--with-parmetis[=ARG] ParMetis install path (contains lib/libparmetis.a)
--with-dirtlib[=ARG] use DiRTlib overset library (contains lib/libdirt.a)
--with-suggar[=ARG] use SUGGAR overset library (contains lib/libsuggar.a)
--with-tecio[=ARG] Tecplot I/O library install path (contains lib/libtecio.a)
--with-refine[=ARG] use refine adaptation package (installation root)
--with-refineFAKEGeom[=ARG] to specify refine FAKEGeom libs [**-lFAUXGeom**]
--with-knife[=ARG] use Knife cut cell package (installation root)
--with-CGNS[=ARG] CGNS library path (installation root)
--with-PORT[=ARG] use PORT optimization library (contains lib/libport.a)
--with-KSOPT[=ARG] use KSOPT optimization library (contains lib/libksopt.a)
--with-SNOPT[=ARG] use SNOPT optimization library (contains lib/libsnopt.a)

Nuts and Bolts (4 of 4)

- FUN3D environment variables of general interest

  `FC` **Fortran compiler command**
  (overridden by `--with-mpif90`)

  `FCFLAGS` **Fortran compiler flags**
  (adds to default unless --disable-ftune)

  `LDFLAGS` **linker flags, e.g. `-L<libdir>`**
  if you have libraries in a nonstandard directory **`<libdir>`**

  `CC` **C compiler command**

  `CFLAGS` **C compiler flags**

  `CXX` **C++ compiler command**

  `CXXFLAGS` **C++ compiler flags**

  `CPPFLAGS` **C/C++ preprocessor flags, e.g. `-I<incdir>`**
  if you have headers in a nonstandard directory **`<incdir>`**

  `CPP` **C preprocessor**

- `make` is used to build the executables
  - Will reside in respective directories (e.g. **`nodet`** is in **`FUN3D_90`**)

Basic Operation

- Construct the *vanilla* **serial** executable
- Unpack your FUN3D distribution
  - Creates a directory "**`fun3d-13.4-454c5d8`**"
- Enter the FUN3D distribution directory
- Run the **`configure`** script and build executables with **`make`**

```
$ mkdir serial
$ cd serial
$ ../configure
$ make
```

- Note that this will search for a supported compiler in your path
- Chooses the first one found based on pre-defined order
- Override this with the **`FC=mycompiler`** option
- MPI configurations will use the **`--with-mpif90`** wrapper if given

Did It Work? Expected Output

```
…
Configuration (FUN3D):
Source code location:..
Version:13.4-454c5d8
Fortran Compiler:  ifort
Fortran basis: ifort
Fortran flags: -O2 -ip –align
  -fno-alias -g -traceback
C Compiler:  gcc
C flags:-g –O2
C++ Compiler:  g++
C++ flags:-g –O2
Linker flags:  –lm
Dependencies:
build:
High Energy Physics: no
Cmplx Variable Tools:no
Python bindings: no
FCCHT support: no
FSI support: no
PDF documentation: yes

bindings:
Libcore:internal
refine: subpackage
CAPRI support: no
```

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```
knife:  subpackage
MPI support:no
CUDA support:  no
Zoltan: no
ParMETIS:  no
Tecplot I/O:no
6DOF libraries:  no
DiRTlib support:no
SUGGAR support:  no
DYMORE support:  no
RCAS_SDX support:  no
CGNS support:  no
PORT support:  no
NPSOL support:no
DOT support:no
KSOPT support:no
SNOPT support:no
SMEMRD support:  version 1.3.1
IRS support:no
SSDC support:  no
SFE support:no
SPARSKIT support:  no
SBOOM support:no
VisIt support:no
```

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- Executables created relative to the *serial* sub-directory
  - **`FUN3D_90/nodet`**, **`Adjoint/dual`**, **`Design/opt_driver`**

Extended Operation

(How we do it)

- Create a **parallel** version of the code
- Build in a separate *configuration* subdirectory
  - Stores object code and executables only
  - Does not pollute the source tree with object code
  - Multiple configurations utilize the same source

```
$ mkdir mpi
$ cd mpi
$ ../configure --with-mpi=/path/to/mpi \
               --with-parmetis=/path/to/parmetis
$ make
```

Did It Work? Expected Output

```
…
Configuration (FUN3D):
Source code location:..
Version:13.4-454c5d8
Fortran Compiler:  /path/to/mpi/bin/mpif90
Fortran basis: ifort
Fortran flags: -O2 -ip –align
  -fno-alias -g -traceback
C Compiler:  /path/to/mpi/bin/mpicc
C flags:-g –O2
C++ Compiler:  g++
C++ flags:-g –O2
Linker flags:  –lm
Dependencies:
build:
High Energy Physics: no
Cmplx Variable Tools:no
Python bindings: no
FCCHT support: no
FSI support: no
PDF documentation: yes

bindings:
Libcore:internal
refine: subpackage
CAPRI support: no
```

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```
knife:  subpackage
MPI support:no
CUDA support:  no
Zoltan: no
ParMETIS: /path/to/parmetis
Tecplot I/O:no
6DOF libraries:  no
DiRTlib support:no
SUGGAR support:  no
DYMORE support:  no
RCAS_SDX support:  no
CGNS support:  no
PORT support:  no
NPSOL support:no
DOT support:no
KSOPT support:no
SNOPT support:no
SMEMRD support:  version 1.3.1
IRS support:no
SSDC support:  no
SFE support:no
SPARSKIT support:  no
SBOOM support:no
VisIt support:no
```

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- Executables created relative to the *mpi* sub-directory
  - **FUN3D_90/nodet**, **Adjoint/dual**, **Design/opt_driver**

Troubleshooting/FAQ (1 of 3)

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- Problems
  - "**`checking for Fortran compiler default output file name... configure: error: Fortran compiler cannot create executables`**
    `See `config.log` for more details`."
  - Make sure that Fortran compiler works in your environment
    - Adjust PATH, load appropriate GNU modules, MPI installation, etc.
  - Limited check of `configure` options
    - Bad "**`--enable-*`**" and "**`--with-*`**" options silently ignored
  - Option values containing spaces must be quoted from shell
    - e.g. **`FCFLAGS="-g -O2 -m32 -fno-common"`**
  - Do **NOT** configure in top level distribution directory and then try to make individual configuration directories
    - **`make distclean`** to clean a previous configuration of the source
  - Look/send "**`config.log`**" file
    - Also includes configuration options at the top (less quoted values w/ spaces)

Troubleshooting/FAQ (2 of 3)

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- Can I…
  - Override the default compiler options?
    - Yes, **`--disable-ftune FCFLAGS="-what-ever-you-want"`**
      - Remember some compilers always need certain options
  - Explicitly specify my compiler?
    - You can, with **`FC=compiler`**, but this will be overridden if using "**`--with-mpif90`**"
  - Fix anything by manually editing the **`configure`** script or Makefiles?
    - **NO**! and we cannot support any such action
    - Anything that you can safely change is governed by a configure option
  - Install the executables in a central location?
    - Yes, **`make install`** will install executables, etc. under the location given by the "**`--prefix=/your/path`**" option to **`configure`**

Troubleshooting/FAQ (3 of 3)

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- What if I…
  - Have a proprietary MPI installation?
    - Some HPC resources have proprietary MPI installations using non-standard paths and names
    - Use "**`--with-mpibin`**", "**`--with-mpiinc`**", "**`--with-mpif90`**", and "**`--with-mpiexec`**" along with their "**`--without-*`**" counterparts as needed to specify the binary and include paths as well as the name for the **`` `mpif90` ``** compiler wrapper and, if needed, the **`` `mpiexec` ``** script
    - Paths can be absolute or relative to the "**`--with-mpi`**" and "**`--with-mpibin`**" values

```
$ ./configure --with-mpi=/path/to/mpi
              --with-mpif90=my_mpif90
              --without-mpiexec
              …
```

  - My MPI executables will not run
    - Check the consistency of your MPI compilation/runtime installations
    - The MPI installation used for compilation is available as MPI Prefix: from

```
$ /path/to/nodet/nodet_mpi --version
```

What We Covered

- How to configure and compile the FUN3D suite
  - Execute `**configure**` to localize a configuration
  - Build the executables with `**make**`
- Configuration options
  - Enable/Disable Features
  - With/Without Packages (3rd party libraries and tools)
  - Custom environment variables
- Use separate configuration subdirectories
  - Keeps source and object code separate
  - Allows multiple configurations under one source
  - Invoke as `**../configure …**`