Utilizing NONMEM 7 and the Intel Fortran Compiler in a Distributed Computing Environment

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Background/Objectives

- With the release of NONMEM 7 (NM7) [1], it is necessary/preferred to compile NONMEM with the Intel fortran compiler (IFC).
- Utilizing IFC in a grid/cluster environment requires the use of the FLEXlm license manager.
- Build on the existing MIfuns R package [3] to develop an open-source method for the deployment of NM7 and IFC in a distributed computing environment.

Problem

NONMEM 7 (NM7) [1] compiled utilizing the Intel fortran compiler (IFC) [2] will be deployed on a computer grid consisting of 4 computers with 8 processing cores per computer. The IFC can be purchased as individual user licenses (∼700/license) or as a cluster license in increments of 5 seats (∼5300/five seat license). The individual user license is meant for a single user machine so installation across a grid is achievable but would be outside of the Intel licensing requirements. NM7 only requires access to a compiler for a brief period of time during the initial compile step so purchasing sufficient cluster seats to accomodate all of the 32 cores would not be cost effective.

Potential Solutions

- Submit each compile/execute job to a machine that is available based on a user check of system load.
- Breakup compile/execute step so compile is accomplished on one machine and execute takes place on another machine or group of machines.
- Implement a queueing system that manages the compile/execute steps and automatically distributes the jobs across a group of machines.

Methods/Implementation

- Required components - NM7, IFC, R, MIfuns, NMQual [5], Sun Grid Engine (SGE) [4], and FLEXlm license manager
- Installation on distributed computing environment (Figure 1)
  1. Perform standard installation of the SGE software on each machine in the grid. Setup a "user-requestable consumable resource" in SGE with a value equal to the number of IFC license seats available. Create at least two cluster queues, all.q (for NONMEM job execution) and compile.q (for NONMEM job compilation). Configure compile.q with the number of slots equal to the number of IFC license seats and all.q with the number of slots equal to or slightly less than the number of available compute cores. (Figure 2)
  2. Install R-2.7.2 or above and the MIfuns R package on each machine in the grid.
  3. Install the FLEXlm license manager on each machine in the grid (one machine will have the license and the other machines will "point" to that license)
  4. Install NM7 with NMQual 7.1.0 on an NFS partition visible across the grid
- Testing
  1. Standard set of 8 control streams in NMQual
  2. Test suite for NM7 that is available in MIfuns
  3. Daily use in a multi-user environment (6 - 8 users)

Figures

Figure 1: *Distributed Computing Workflow*

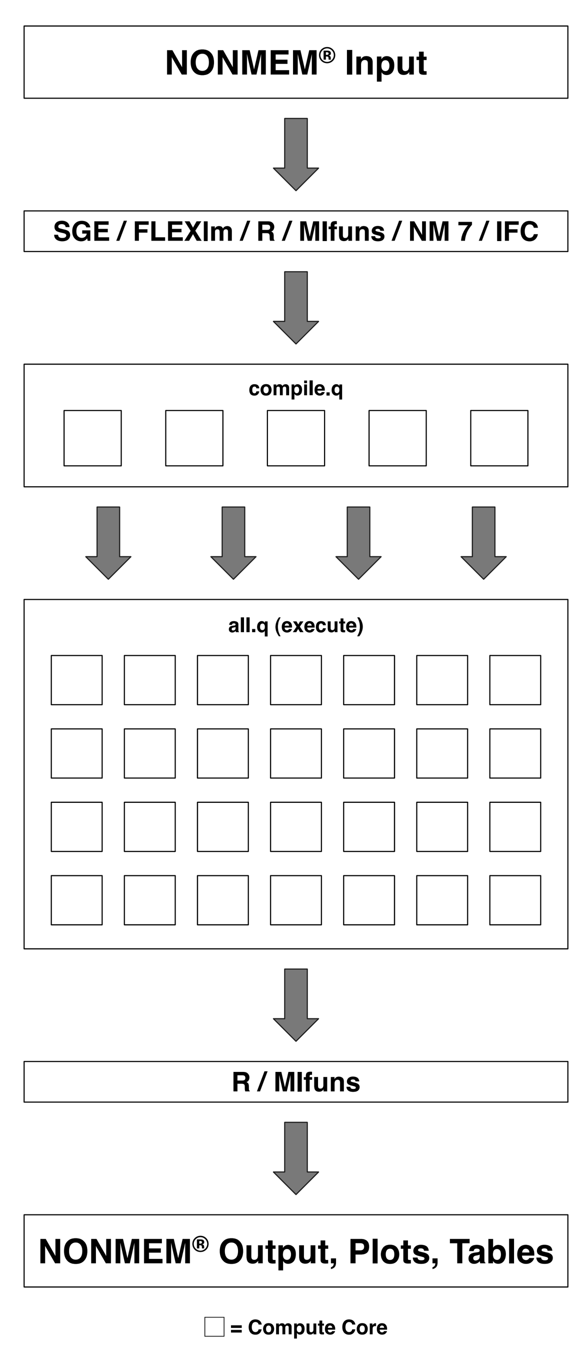

Figure 2: *SGE Queue Setup*

queue	qtype	used/tot.	load_avg	arch	states
all.q@host01	BIP	0/7	1.04	darwin-x86	
36 0.56 Run5e	billk	r	6/1/10	14:10:55	1
37 0.56 Run6e	billk	r	6/1/10	10:09:53	1
all.q@host02	BIP	0/7	1.02	darwin-x86	
35 0.56 Run1e	billk	r	5/31/10	9:09:01	1
all.q@host03	BIP	0/7	1.54	darwin-x86	
all.q@host04	BIP	0/7	1.03	darwin-x86	
compile.q@host01	BIP	0/2	1.04	darwin-x86	
38 0.56 Run7c	billk	r	6/1/10	14:12:53	1
compile.q@host02	BIP	0/2	1.02	darwin-x86	
39 0.56 Run8c	billk	r	6/1/10	14:12:55	1
compile.q@host03	BIP	0/1	1.54	darwin-x86	

Results

- All tests ran successfully.
- When number of submitted "compile" jobs exceeded five, the remaining jobs were held by SGE until an IFC license was available.

Conclusions

- No discernible time difference when NONMEM job was split into compile and execute portions using SGE versus running the NONMEM job outside of SGE.
- Limiting number of IFC seats to 5 resulted in cost savings versus buying 1 IFC seat/CPU core.
- Successful distribution of NM7 jobs in a multi-user, grid environment.
- Successful utilization of open-source software (R, SGE, MIfuns, NMQual) to maximize grid utilization and minimize cost.

References

[1] NONMEM VI and 7, ICON Development Solutions, Ellicott City, MD, USA

[2] Intel Fortran Compiler, Intel Corporation, Santa Clara, CA, USA

[3] Facilitating the Pharmacometrics Work-Flow with the MItools R Package, ACOP 2009, Tuscon, AZ

[4] Sun Microsystems, http://gridengine.sunsource.net/

[5] NONMEM Installation with NMQual, Metrum Institute, Tariffville, CT, USA

Appendix: Example function calls for MIfuns and SGE

NONR() call to run NM7 on grid

```
NONR(run=c(5,6,7,8),
     command="/com/NONMEM/nm7osx1/test/
       nm7osx1",
     project=ProjectDir,
     grid=TRUE,
     diag=TRUE,
     covplt=TRUE,
     cat.cov=c("SEX","RACE"),
     cont.cov=c("AGE","WT","BMI"),
     par.list=c("CL","V","KA"),
     eta.list=c("ETA1","ETA2","ETA3")
     )
```

qstat call to generate output for Figure 2

```
qstat -f
```

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