## Compiling your own software at Prince

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Running jobs on the Prince Cluster

Accessing the Prince Cluster

- From Windows workstation
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Software and Environment Module

Job script and resource request

- Introduction to job scheduling
- Submitting jobs with sbatch
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Canceling your jobs

Compiling your own software

Putting all pieces together

- An Amber example
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Summary

Compiling Code for Prince

We recommend using the Intel compiler suite (module spider intel), and, for MPI programs, OpenMPI (module spider openmpi/intel).

The GNU compiler suite is also available (module spider gcc) and over time other compiler versions and MPI implementations will be installed. There will be instances in which an alternative compiler or MPI library performs better or avoids a bug in the recommended compilers, but in the long run the functionality and performance of compilers and MPI libraries is very similar, so for easiest maintenance, only use the alternatives if you really need to.

For the best performance, you should compile your code optimized with AVX2 vector instructions for faster floating point computations, also to generate multi-threaded code based on the OpenMP* directives. To do so, use the following flags to icc, icpc and ifort:

```
-O3 -fPIC -unroll -ip -axCORE-AVX2 -qopenmp -qopt-report-stdout -qopt-report-phase=openmp
```

For the link step, you can add a flag "-shared-intel".

If you need GNU compilers, we recommend enabling AVX and disabling AVX2 instructions to ensure your executable can run on any compute nodes. To do this add the flag:

```
-mavx -mno-avx2
```
AVX2 vectorize loops, meaning that several iterations of the loop are executed concurrently. This changes the order of operations, which can change the results. Programs using summations over loops are especially vulnerable to this.

Many algorithms and problems are numerically sensitive, and vectorization or certain aggressive optimizations can be enough to trigger numerical instability. Debugging numerical instability is complex. Intel has some interesting information about it here but if you suspect your model is experiencing it you should disable vectorization, use \texttt{-fp-model precise} or \texttt{-fp-model strict} and reduce optimization flags from \texttt{-O3} to \texttt{-O2} or \texttt{-O0}, and use this as a baseline to test higher levels of optimization.

If you are building software to use for many or long-running jobs, testing for performance with a few MPI libraries and compile options can be very valuable since a specific model might run noticeably faster under one MPI implementation than another.