National Supercomputing Centre

Applications: Spack and Gromacs

26 July 2022

Dr Jernej Zidar,
Senior HPC Application Analyst
jernej@nscc.sg

What is Spack?

- Package manager for HPC systems
- Aim:
  - Simplify deployments of applications
  - Provide a framework that allows to mix & match various versions of compilers, MPI, scientific libraries in a systematic and reproducible way

Installation and Setup

```
[zidarj1@asp2a-login012 ~]$ git clone -c feature.manyFiles=true https://github.com/spack/spack.git spack
Cloning into 'spack'...
remote: Enumerating objects: 394360, done.
remote: Counting objects: 100% (140/140), done.
remote: Compressing objects: 100% (104/104), done.
remote: Total 394360 (delta 48), reused 87 (delta 16), pack-reused 394220
Receiving objects: 100% (394360/394360), 176.66 MiB | 16.42 MiB/s, done.
Resolving deltas: 100% (170203/170203), done.
Updating files: 100% (9593/9593), done.
[zidarj1@asp2a-login012 ~]$
```

```
[zidarj1@asp2a-login012 ~]$ spack compilers
==> Available compilers
-- aocc rhel8-any ------------------------------------------------
aocc@3.2.0

-- cce rhel8-any -------------------------------------------------
cce@13.0.2

-- gcc rhel8-any -------------------------------------------------
gcc@12.1.0-nscc  gcc@11.3.0-nscc  gcc@11.2.0-nscc  gcc@11.2.0  gcc@10.3.0  gcc@8.5.0-nscc  gcc@8.1.0

-- intel rhel8-any -----------------------------------------------
intel@2022.0.2

-- nvhpc rhel8-any -----------------------------------------------
nvhpc@22.5  nvhpc@22.3
[zidarj1@asp2a-login012 ~]$
```

Installed compilers are automatically detected.

Install a Simple Package

1. Check what should be installed using `spack spec …`

```
[zidarj1@asp2a-login012 ~]$ spack spec gromacs%gcc
Input spec
--------------------------------
gromacs%gcc

Concretized
--------------------------------
gromacs@2022.2%gcc@11.2.0~blas~cuda~cycle_subcounters~double+hwloc~ipo~lapack~mdrun_only+mpi~nosuffix~opencl+openmp~plumed~re
laxed_double_precision+shared~sycl build_type=RelWithDebInfo arch=cray-rhel8-zen3
    ^cmake@3.18.2%gcc@11.2.0~doc+ncurses+ownlibs~qt build_type=Release patches=bf695e3 arch=cray-rhel8-zen3
    ^cray-fftw@3.3.8.13%gcc@11.2.0+mpi~openmp precision=double,float arch=cray-rhel8-zen3
    ^cray-mpich@8.1.15%gcc@11.2.0+wrappers arch=cray-rhel8-zen3
    ^hwloc@2.7.1%gcc@11.2.0~cairo~cuda~gl~libudev+libxml2~netloc~nvml~oneapi-level-zero~opencl+pci~rocm+shared arch=cray-rhel
8-zen3
        ^libpciaccess@0.16%gcc@11.2.0 arch=cray-rhel8-zen3
            ^libtool@2.4.6%gcc@11.2.0 arch=cray-rhel8-zen3
            ^pkgconf@1.4.2%gcc@11.2.0 arch=cray-rhel8-zen3
            ^util-macros@1.19.3%gcc@11.2.0 arch=cray-rhel8-zen3
        ^libxml2@2.9.13%gcc@11.2.0~python arch=cray-rhel8-zen3
            ^libiconv@1.16%gcc@11.2.0 libs=shared,static arch=cray-rhel8-zen3
            ^xz@5.2.5%gcc@11.2.0~pic libs=shared,static arch=cray-rhel8-zen3
            ^zlib@1.2.12%gcc@11.2.0+optimize+pic+shared patches=0d38234 arch=cray-rhel8-zen3
        ^ncurses@6.2%gcc@11.2.0~symlinks+termlib abi=none arch=cray-rhel8-zen3

[zidarj1@asp2a-login012 ~]$
```

2. Install the package using `spack install …`

Use a Simple Package

Installed packages are available as modules on compute nodes

```
[zidarj1@x1001c0s2b0n0 ~]$ gmx_mpi --version
                      :-) GROMACS - gmx_mpi, 2022.2-spack (-:

Executable:   /scratch/users/astar/bmsi/zidarj1/app/spack/opt/spack/cray-rhel8-zen3/gcc-11.2.0/gromacs-2022.2-26tck6c5fursz2mt6ur5
xiwoujat55hv/bin/gmx_mpi
Data prefix:  /scratch/users/astar/bmsi/zidarj1/app/spack/opt/spack/cray-rhel8-zen3/gcc-11.2.0/gromacs-2022.2-26tck6c5fursz2mt6ur5
xiwoujat55hv
Working dir:  /scratch/GPFS/home/users/astar/bmsi/zidarj1
Command line:
  gmx_mpi --version

GROMACS version:    2022.2-spack
Precision:          mixed
Memory model:       64 bit
MPI library:        MPI
OpenMP support:     enabled (GMX_OPENMP_MAX_THREADS = 128)
GPU support:        disabled
SIMD instructions:  AVX2_256
CPU FFT library:    commercial-fftw-3.3.8-sse2-avx-avx2-avx2_128
GPU FFT library:    none
RDTSCP usage:       enabled
TNG support:        enabled
Hwloc support:      hwloc-2.7.1
Tracing support:    disabled
C compiler:         /scratch/users/astar/bmsi/zidarj1/app/spack/lib/spack/env/gcc/gcc GNU 11.2.0
C compiler flags:   -mavx2 -mfma -Wno-missing-field-initializers -fexcess-precision=fast -funroll-all-loops -O2 -g -DNDEBUG
C++ compiler:       /scratch/users/astar/bmsi/zidarj1/app/spack/lib/spack/env/gcc/g++ GNU 11.2.0
C++ compiler flags: -mavx2 -mfma -Wno-missing-field-initializers -fexcess-precision=fast -funroll-all-loops -fopenmp -O2 -g -DNDEB
UG
```

Use a Simple Package

```
[zidarj1@x1001c0s2b0n0 ~]$ aprun gmx_mpi mdrun -h
                  :-) GROMACS - gmx mdrun, 2022.2-spack (-:

Executable:   /var/run/palsd/000b322d-1b1f-4f9b-adf1-e3d0f386084b/files/gmx_mpi
Data prefix:  /scratch/users/astar/bmsi/zidarj1/app/spack/opt/spack/cray-rhel8-zen3/gcc-11.2.0/gromacs-2022.2-26tck6c5fursz2mt6ur5
xiwoujat55hv
Working dir:  /scratch/GPFS/home/users/astar/bmsi/zidarj1
Command line:
  gmx_mpi mdrun -h

SYNOPSIS

gmx mdrun [-s [<.tpr>]] [-cpi [<.cpt>]] [-table [<.xvg>]] [-tablep [<.xvg>]]
          [-tableb [<.xvg> [...]]] [-rerun [<.xtc/.trr/...>]] [-ei [<.edi>]]
          [-multidir [<dir> [...]]] [-awh [<.xvg>]] [-membed [<.dat>]]
          [-mp [<.top>]] [-mn [<.ndx>]] [-o [<.trr/.cpt/...>]]
          [-x [<.xtc/.tng>]] [-cpo [<.cpt>]] [-c [<.gro/.g96/...>]]
          [-e [<.edr>]] [-g [<.log>]] [-dhdl [<.xvg>]] [-field [<.xvg>]]
          [-tpi [<.xvg>]] [-tpid [<.xvg>]] [-eo [<.xvg>]] [-px [<.xvg>]]
          [-pf [<.xvg>]] [-ro [<.xvg>]] [-ra [<.log>]] [-rs [<.log>]]
          [-rt [<.log>]] [-mtx [<.mtx>]] [-if [<.xvg>]] [-swap [<.xvg>]]
          [-deffnm <string>] [-xvg <enum>] [-dd <vector>] [-ddorder <enum>]
          [-npme <int>] [-nt <int>] [-ntmpi <int>] [-ntomp <int>]
          [-ntomp_pme <int>] [-pin <enum>] [-pinoffset <int>]
          [-pinstride <int>] [-gpu_id <string>] [-gputasks <string>]
          [-[no]ddcheck] [-rdd <real>] [-rcon <real>] [-dlb <enum>]
          [-dds <real>] [-nb <enum>] [-nstlist <int>] [-[no]tunepme]
          [-pme <enum>] [-pmefft <enum>] [-bonded <enum>] [-update <enum>]
          [-[no]v] [-pforce <real>] [-[no]reprod] [-cpt <real>] [-[no]cpnum]
          [-[no]append] [-nsteps <int>] [-maxh <real>] [-replex <int>]
          [-nex <int>] [-reseed <int>]

DESCRIPTION

gmx mdrun is the main computational chemistry engine within GROMACS.
Obviously, it performs Molecular Dynamics simulations, but it can also perform
Stochastic Dynamics, Energy Minimization, test particle insertion or
(re)calculation of energies. Normal mode analysis is another option. In this
case mdrun builds a Hessian matrix from single conformation. For usual Normal
Modes-like calculations, make sure that the structure provided is properly
energy-minimized. The generated matrix can be diagonalized by gmx nmeig.
```

However…

```
 not unique to Intel microprocessors
==> Using cached archive: /scratch/users/astar/bmsi/zidarj1/app/spack/var/spack/cache/_source-cache/archive/65/656404f884d2fa2244c
97d2a5b92af148d0dbea94ad13004724b3fcbf45e01bf.tar.gz
==> Ran patch() for gromacs
==> gromacs: Executing phase: 'cmake'
==> Error: ProcessError: Command exited with status 1:
    'cmake' '-G' 'Unix Makefiles' '-DCMAKE_INSTALL_PREFIX:STRING=/scratch/users/astar/bmsi/zidarj1/app/spack/opt/spack/cray-rhel8-
zen3/intel-2022.0.2/gromacs-2022.2-pvuof7he3iku2hjyfx3sghlev7hlxsg3' '-DCMAKE_BUILD_TYPE:STRING=RelWithDebInfo' '-DBUILD_TESTING:B
OOL=OFF' '-DCMAKE_INTERPROCEDURAL_OPTIMIZATION:BOOL=OFF' '-DCMAKE_VERBOSE_MAKEFILE:BOOL=ON' '-DCMAKE_INSTALL_RPATH_USE_LINK_PATH:B
OOL=ON' '-DCMAKE_INSTALL_RPATH:STRING=/scratch/users/astar/bmsi/zidarj1/app/spack/opt/spack/cray-rhel8-zen3/intel-2022.0.2/gromacs
-2022.2-pvuof7he3iku2hjyfx3sghlev7hlxsg3/lib;/scratch/users/astar/bmsi/zidarj1/app/spack/opt/spack/cray-rhel8-zen3/intel-2022.0.2/
gromacs-2022.2-pvuof7he3iku2hjyfx3sghlev7hlxsg3/lib64;/opt/cray/pe/fftw/3.3.8.13/x86_rome/lib;/opt/cray/pe/mpich/8.1.15/ofi/intel/
19.0/lib;/scratch/users/astar/bmsi/zidarj1/app/spack/opt/spack/cray-rhel8-zen3/intel-2022.0.2/hwloc-2.7.1-lpf3b4mtcktedl73lpt4zbiq
3hjahytl/lib;/scratch/users/astar/bmsi/zidarj1/app/spack/opt/spack/cray-rhel8-zen3/intel-2022.0.2/libpciaccess-0.16-a6mmn6kx5zb5wa
pp5plhovfubfy4sjhi/lib;/scratch/users/astar/bmsi/zidarj1/app/spack/opt/spack/cray-rhel8-zen3/intel-2022.0.2/libxml2-2.9.13-3xadypr
tko6m47iofum6qerzobqw5nrf/lib;/scratch/users/astar/bmsi/zidarj1/app/spack/opt/spack/cray-rhel8-zen3/intel-2022.0.2/libiconv-1.16-z
qdie6fb5uartozptvkxgydrxulbvnhp/lib;/scratch/users/astar/bmsi/zidarj1/app/spack/opt/spack/cray-rhel8-zen3/intel-2022.0.2/xz-5.2.5-
c6t6gios6kmbne25hgawqw3kjlac3a6r/lib;/scratch/users/astar/bmsi/zidarj1/app/spack/opt/spack/cray-rhel8-zen3/intel-2022.0.2/zlib-1.2
.12-mfcxqvgjl56expou6vh3xowpvekawn5b/lib;/scratch/users/astar/bmsi/zidarj1/app/spack/opt/spack/cray-rhel8-zen3/intel-2022.0.2/ncur
ses-6.2-jfol6ocqfoynmkb66aaz6qgvn4jdctjg/lib;/app/apps/oneapi/2022.1.2/compiler/2022.0.2/linux' '-DCMAKE_PREFIX_PATH:STRING=/scrat
ch/users/astar/bmsi/zidarj1/app/spack/opt/spack/cray-rhel8-zen3/intel-2022.0.2/hwloc-2.7.1-lpf3b4mtcktedl73lpt4zbiq3hjahytl;/scrat
ch/users/astar/bmsi/zidarj1/app/spack/opt/spack/cray-rhel8-zen3/intel-2022.0.2/ncurses-6.2-jfol6ocqfoynmkb66aaz6qgvn4jdctjg;/scrat
ch/users/astar/bmsi/zidarj1/app/spack/opt/spack/cray-rhel8-zen3/intel-2022.0.2/libxml2-2.9.13-3xadyprtko6m47iofum6qerzobqw5nrf;/sc
ratch/users/astar/bmsi/zidarj1/app/spack/opt/spack/cray-rhel8-zen3/intel-2022.0.2/zlib-1.2.12-mfcxqvgjl56expou6vh3xowpvekawn5b;/sc
ratch/users/astar/bmsi/zidarj1/app/spack/opt/spack/cray-rhel8-zen3/intel-2022.0.2/xz-5.2.5-c6t6gios6kmbne25hgawqw3kjlac3a6r;/scrat
ch/users/astar/bmsi/zidarj1/app/spack/opt/spack/cray-rhel8-zen3/intel-2022.0.2/libiconv-1.16-zqdie6fb5uartozptvkxgydrxulbvnhp;/scr
atch/users/astar/bmsi/zidarj1/app/spack/opt/spack/cray-rhel8-zen3/intel-2022.0.2/libpciaccess-0.16-a6mmn6kx5zb5wapp5plhovfubfy4sjh
i;/opt/cray/pe/mpich/8.1.15/ofi/intel/19.0;/opt/cray/pe/fftw/3.3.8.13/x86_rome' '-DGMX_MPI:BOOL=ON' '-DCMAKE_C_COMPILER=/scratch/u
sers/astar/bmsi/zidarj1/app/spack/lib/spack/env/intel/icc' '-DCMAKE_CXX_COMPILER=/scratch/users/astar/bmsi/zidarj1/app/spack/lib/s
pack/env/intel/icpc' '-DMPI_C_COMPILER=/opt/cray/pe/mpich/8.1.15/ofi/intel/19.0/bin/mpicc' '-DMPI_CXX_COMPILER=/opt/cray/pe/mpich/
8.1.15/ofi/intel/19.0/bin/mpicxx' '-DGMX_INSTALL_LEGACY_API=ON' '-DGMX_HWLOC:BOOL=ON' '-DGMX_GPU:STRING=OFF' '-DGMX_EXTERNAL_LAPAC
K:BOOL=OFF' '-DGMX_EXTERNAL_BLAS:BOOL=OFF' '-DGMX_SIMD=AVX2_256' '-DGMX_USE_RDTSCP:BOOL=ON' '-DGMX_OPENMP:BOOL=ON' '-DGMX_CYCLE_SU
BCOUNTERS:BOOL=OFF' '-DGMX_FFT_LIBRARY=fftw3' '-DGMX_VERSION_STRING_OF_FORK=spack' '/tmp/zidarj1/spack-stage/spack-stage-gromacs-2
022.2-pvuof7he3iku2hjyfx3sghlev7hlxsg3/spack-src'

1 error found in build log:
     102    -- Check if the system is big endian - little endian
     103    -- MPI is not compatible with thread-MPI. Disabling thread-MPI.
     104    -- Could NOT find MPI_CXX (missing: MPI_CXX_LIB_NAMES) (found version "3.1")
     105    -- Could NOT find MPI (missing: MPI_CXX_FOUND CXX) (found version "3.1")
     106        Reason given by package: MPI component 'Fortran' was requested, but language Fortran is not enabled.
     107
  >> 108    CMake Error at cmake/gmxManageMPI.cmake:71 (message):
     109      MPI support requested, but no suitable MPI compiler found.  Either set the
     110      MPI_CXX_COMPILER to the MPI compiler wrapper (often called mpicxx or
     111      mpic++), set CMAKE_CXX_COMPILER to a default-MPI-enabled compiler, or set
     112      the variables reported missing for MPI_CXX above.
     113    Call Stack (most recent call first):
     114      CMakeLists.txt:422 (include)

See build log for details:
  /tmp/zidarj1/spack-stage/spack-stage-gromacs-2022.2-pvuof7he3iku2hjyfx3sghlev7hlxsg3/spack-build-out.txt
```

Some Final Thoughts About Spack

- With three different families of compilers, three different sets of math libraries on ASPIRE2A, Spack could greatly simplify the management of the software stack
- The good: users can install their own software
- The bad: every piece of software needs a specific build recipe
- Next steps: continued evaluation by NSCC Software Team

What is Gromacs?

- Molecular dynamics package
- Aim:
  - Prepare and run molecular dynamics simulations
  - Analyze trajectory data

Gromacs Performance Benchmarks

- Reminder: each ASPIRE2A node has 128 cores
- Performance depends on:
  - Compiler, MPI library and math library used to compile the executable
  - Size and shape of the simulated biomolecular system
  - Number of nodes/cores/accelerators used for the simulation

Gromacs Performance Benchmarks (cont.)

Compiler	MPI	Math Library
CCE 13.0.2	cray-mpich	Lib-sci
GCC 11.2.0		Lib-sci
Intel 2022.0.2		MKL

Cray MPICH is recommended by the vendor.

Gromacs Performance Benchmarks (cont.)

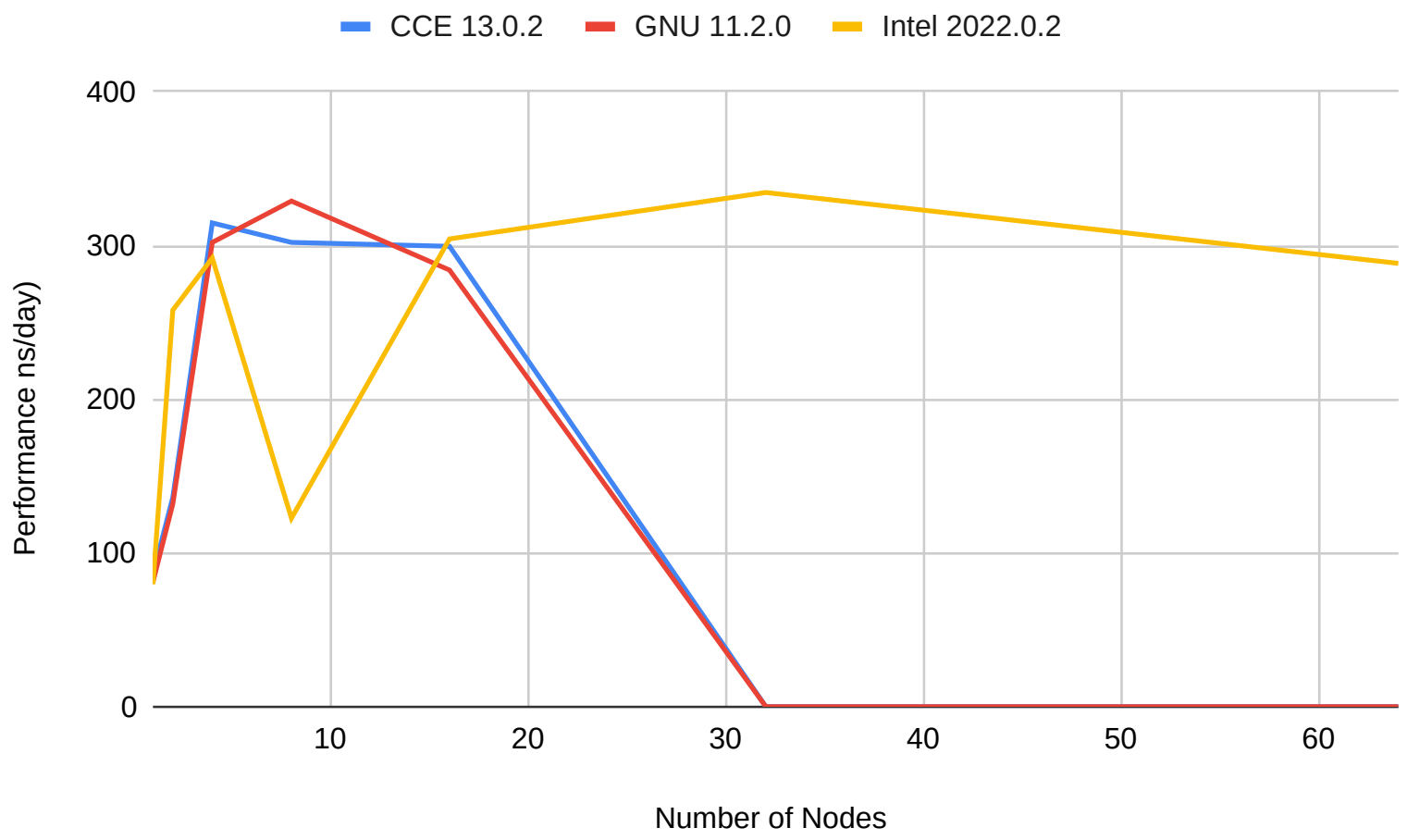
Label	Description	Size (x y z, nm)	Number of Atoms
ION	Ion Channel	11.2 x 9.7 x 14.8	141,677
STMV	Satellite Tobacco Mosaic Virus	21.7 x 21.7 x 21.7	1,066,628
PEP	Peptides	50 x 50 x 50	12,495,503

Gromacs Performance Benchmarks (cont.)

1. Run details:
    1. For each benchmark execute 5 runs
    2. Execute benchmarks on 1, 2, 4, 8, 16, 32, 64, 128, 256 nodes
    3. Use Gromacs 2022.2 executables compiled either with CCE 13.0.2, GNU 11.2.0 or Intel 2022.0.2 compilers using Cray MPICH for MPI
2. Data processing:
    1. Collect performance data
    2. Compute average, standard deviation
    3. Compute speed-up and parallel efficiency

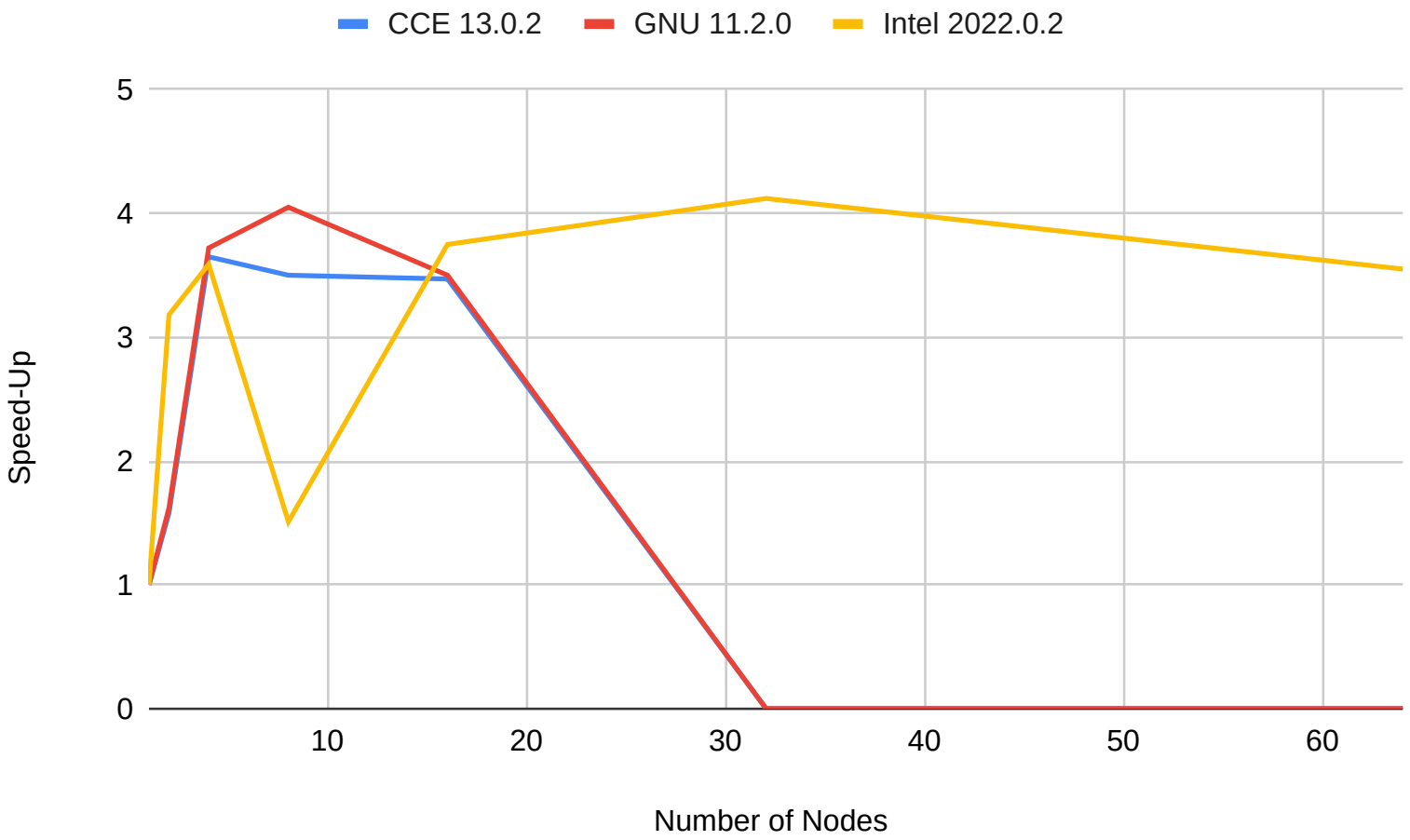
Gromacs Performance Benchmarks (cont.)

1. ION



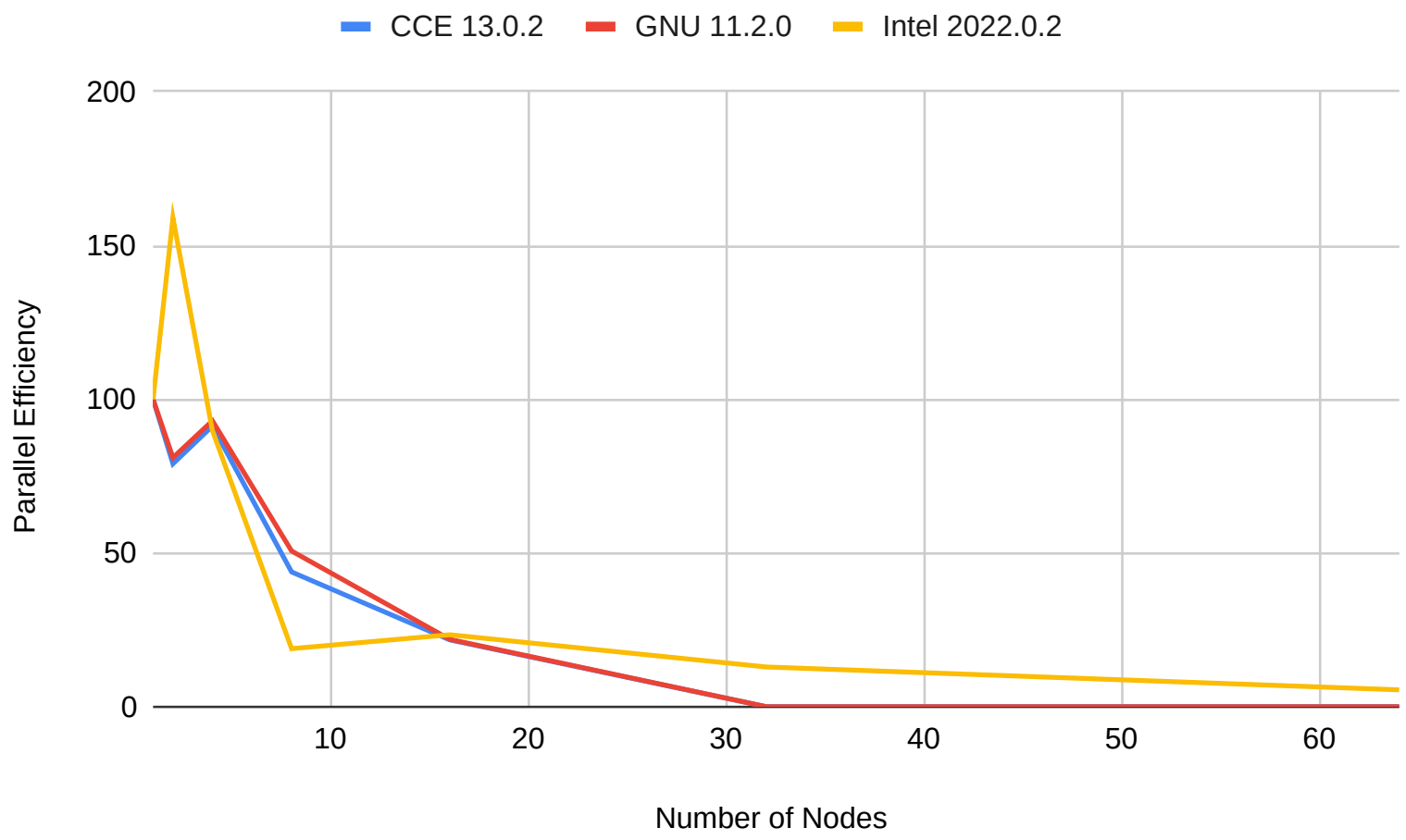
Gromacs Performance Benchmarks (cont.)

1. ION



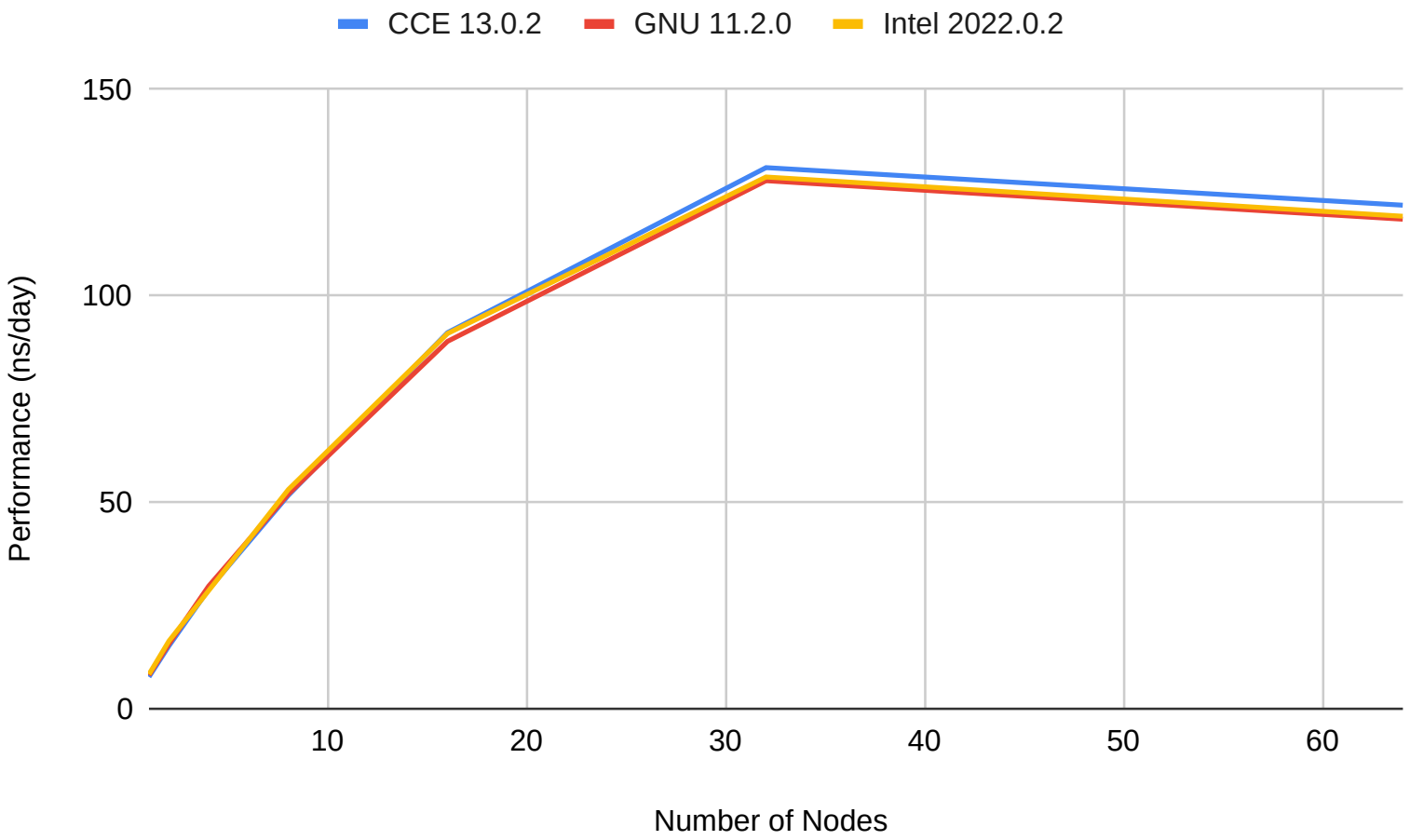
Gromacs Performance Benchmarks (cont.)

1. ION



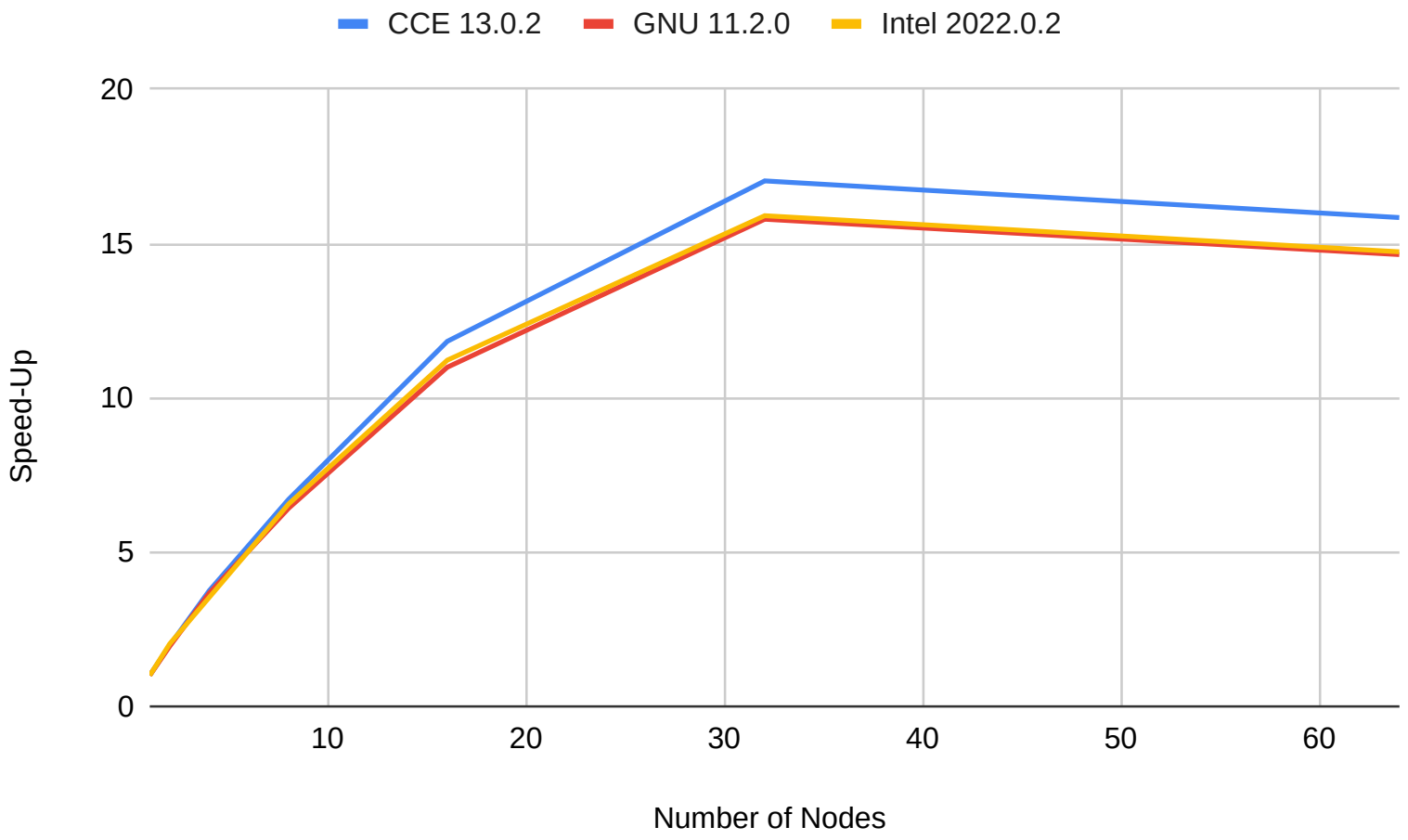
Gromacs Performance Benchmarks (cont.)

2. STMV



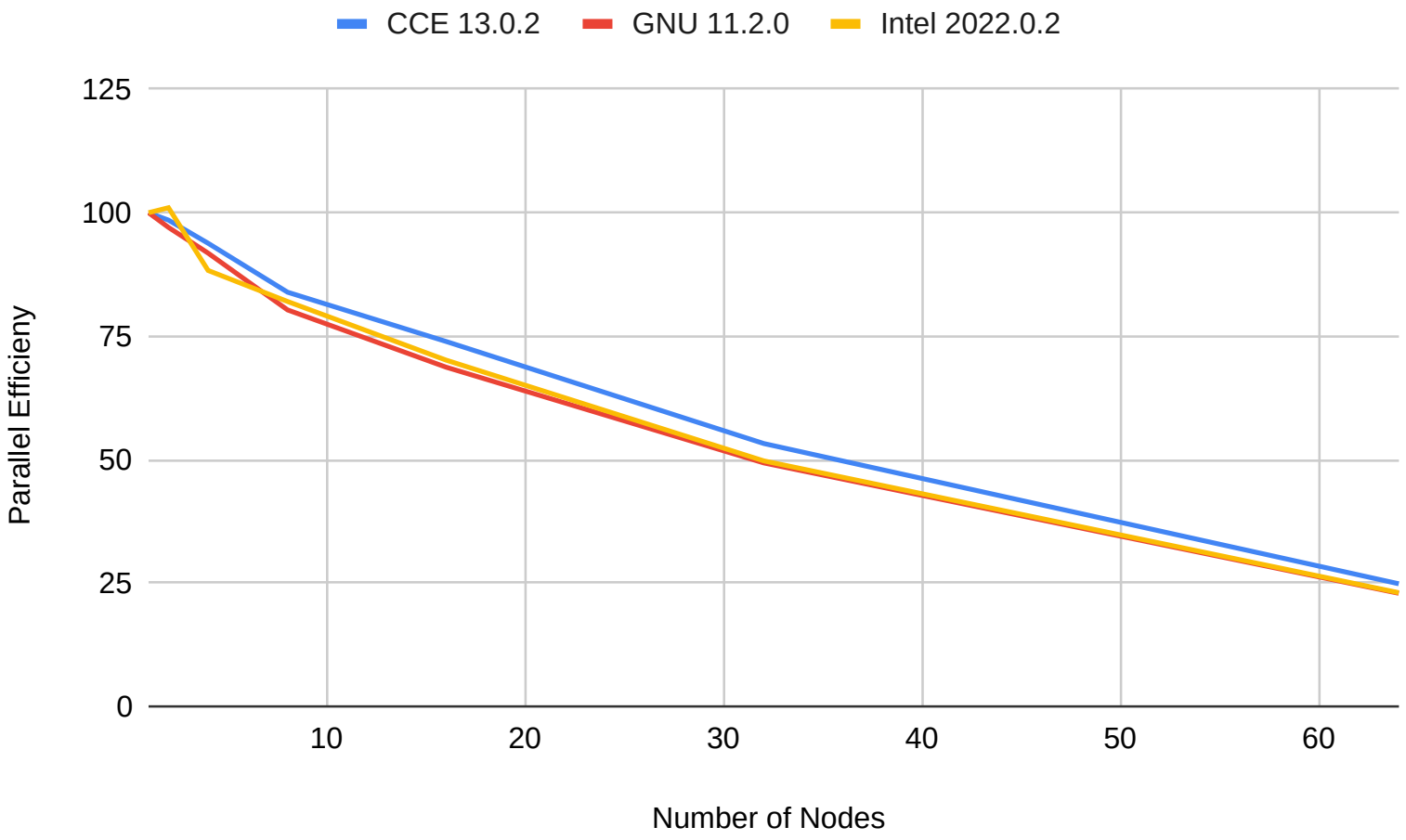
Gromacs Performance Benchmarks (cont.)

2. STMV



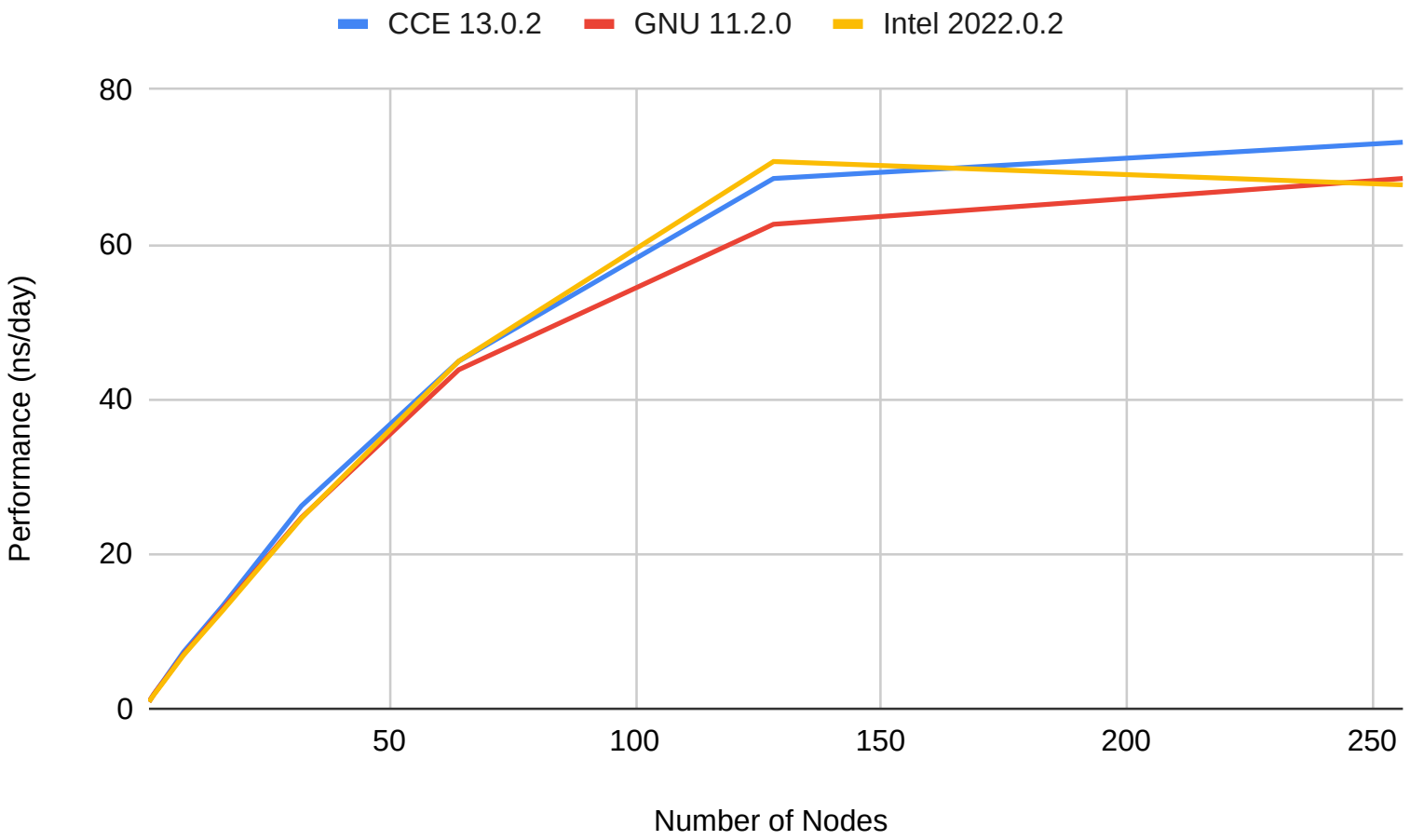
Gromacs Performance Benchmarks (cont.)

2. STMV



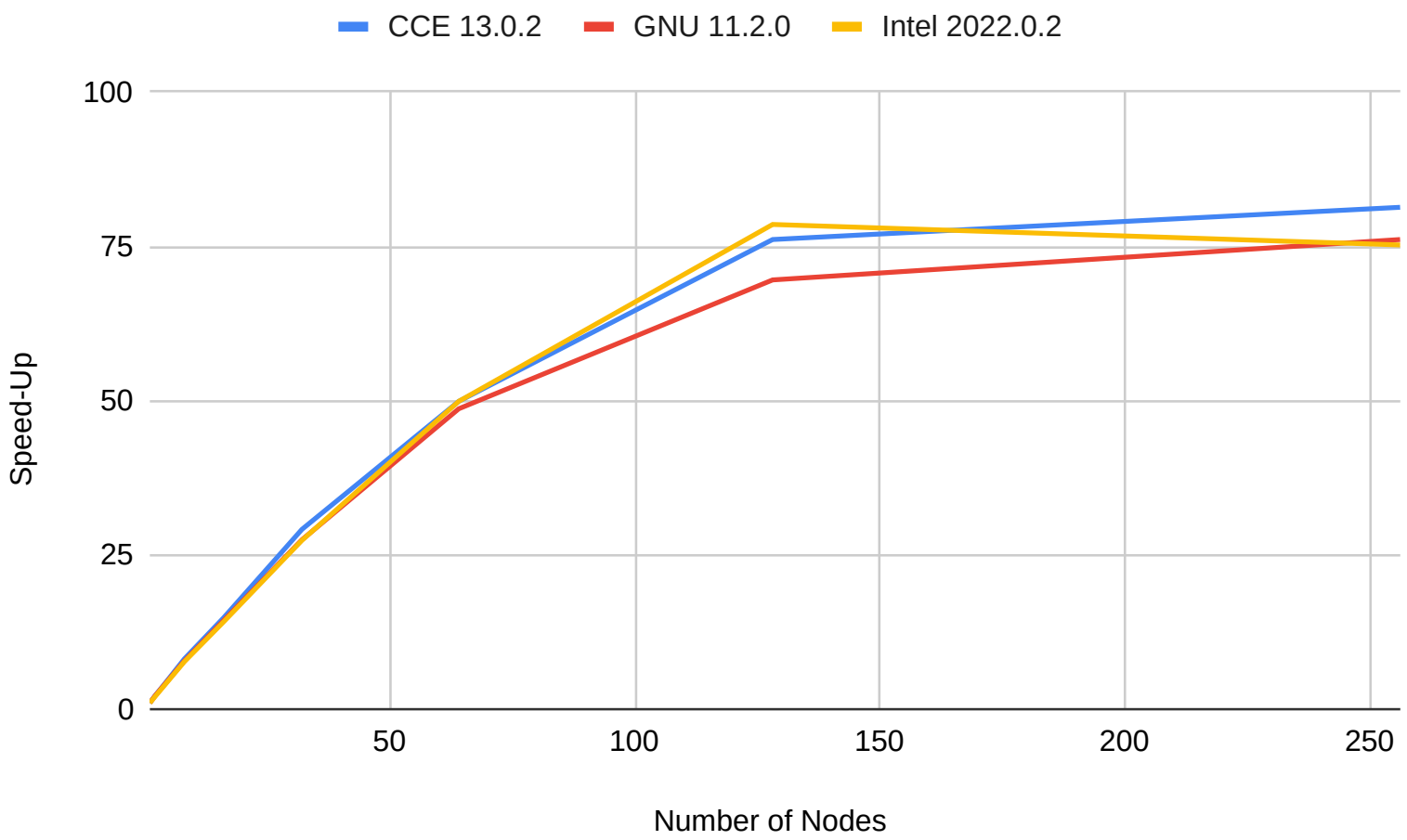
Gromacs Performance Benchmarks (cont.)

3. PEP



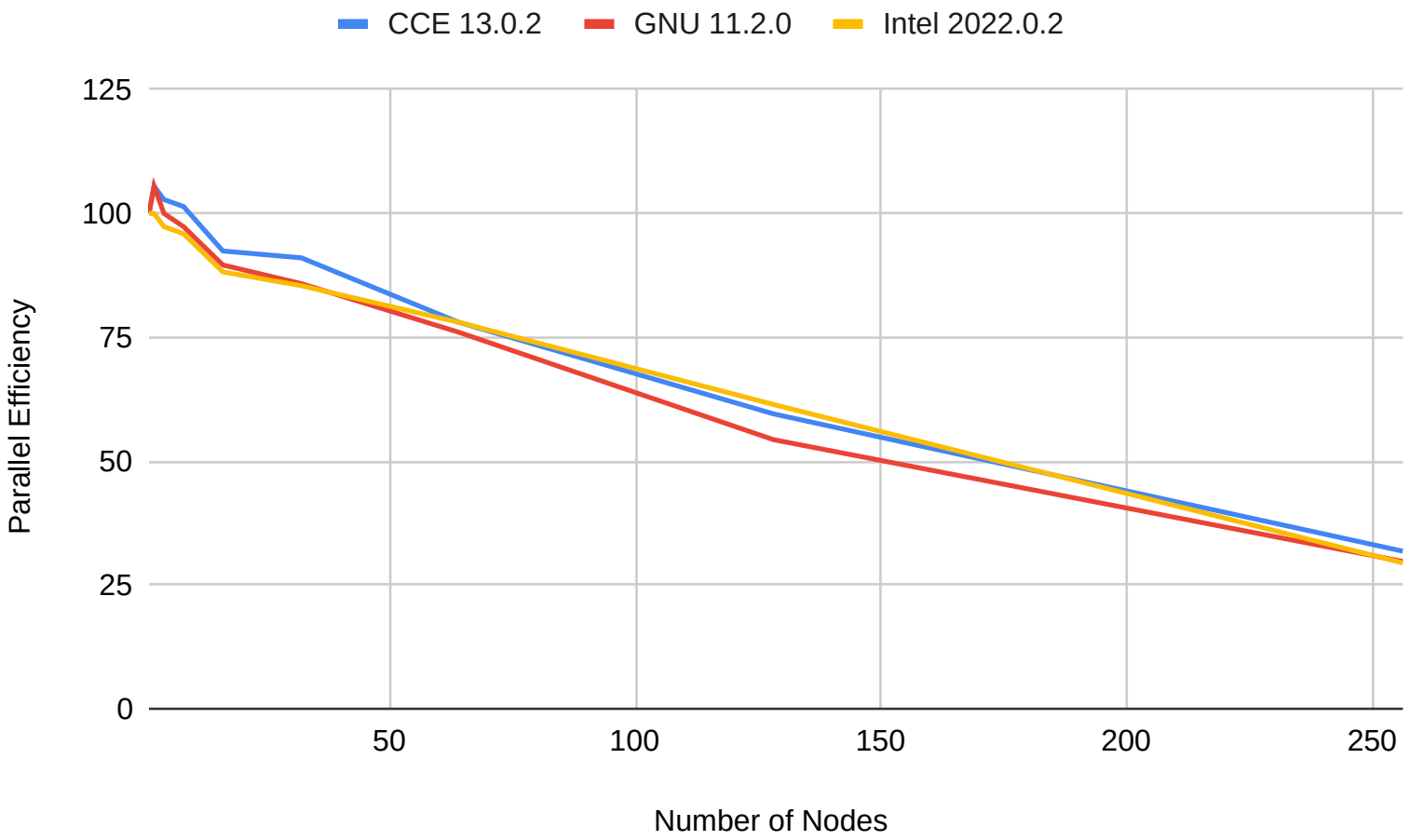
Gromacs Performance Benchmarks (cont.)

3. PEP



Gromacs Performance Benchmarks (cont.)

3. PEP



Some Final Thoughts About Gromacs

- For small systems (~100k atoms) up to 8 nodes will likely get the best performance
- For medium sized systems (~1M) 32 nodes should gave the best performance
- For large systems (>12M) up to 128 nodes could be used
- Best performance is obtained with either GNU or Intel compilers
- Users are invited to perform a few short runs (~15 minutes walltime) using different number of compute nodes to determine the optimal amount of resources required
- More resources consumed may not result in better performance

National Supercomputing Centre

Thank You

NSCC.SG