

Gromacs Code(1) – SIMD

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Introduction

- Most time-consuming function
- File generator and the generated function
- Basic work flow

Most Time-consuming Function

- According to the *gprof* result:
 - `nbnxn_kernel_ElecEw_VdwLJCombLB_F_2xnn` is the most time-consuming function;
 - its name suggests that this function is *generated automatically*
- Now we need to find out 2 things:
 - **where** are those generated functions and **which** file is their original template
 - what about its **functionality** and how could we improve its performance?

Where is it?

- Path:
 - gromacs-5.0.2 ▶ src ▶ gromacs ▶ **mdlib** ▶ nbnnxn_kernels
 - it suggests that this function is a molecule dynamic kernel calculating function
- nbnnxn_kernels:
 - in this directory, there're 2 kinds of files:
 1. basic c & CUDA routines for md calculation
 2. 1 **file generator** and 2 directories containing the **generated functions**
 3. Now we need to find out the original template

File Generator (1) – Translate

- In the file generator directory, there're 4 c code template and 1 python script
 - after translated that python script, we could know what's that time-consuming function is about
- `nbnxn_kernel_ElecEw_VdwLJCombLB_F_2xnn`
 - “`nbnxn_kernel_`” is a common prefix
 - “`ElecEw`” specifies the **Electrostatics**
 - “`VdwLJCombLB`” is a property of **VdwTreatment** which I don't understand
 - “`F`” means this function will not calculate energy
 - “`2xnn`” means this function will use 8 or 16 width SIMD instructions

File Generator (2) – Generated

pre-defined

```
#define GMX_SIMD_J_UNROLL_SIZE 2
#include "nbnxn_kernel_simd_2xnn.h"

#define CALC_COUL_EWALD
#define LJ_CUT
#define LJ_COMB_LB
/* Will not calculate energies */

#ifdef GMX_NBNXN_SIMD_2XNN
#include "nbnxn_kernel_simd_2xnn_common.h"
#endif /* GMX_NBNXN_SIMD_2XNN */
```

function body

```
#ifdef GMX_NBNXN_SIMD_2XNN
#include "nbnxn_kernel_simd_2xnn_outer.h"
#else /* GMX_NBNXN_SIMD_2XNN */
{
/* No need to call gmx_incons() here, because the only function
 * that calls this one is also compiled conditionally. When
 * GMX_NBNXN_SIMD_2XNN is not defined, it will call no kernel functions and
 * instead call gmx_incons().
 */
}
#endif /* GMX_NBNXN_SIMD_2XNN */
```

function declaration

```
#ifdef CALC_ENERGIES
void
nbnxn_kernel_ElecEw_VdwLJCombLB_F_2xnn(const nbnxn_pairlist_t
                                       const nbnxn_atomdata_t
                                       const interaction_const_t
                                       rvec
                                       real
                                       real
                                       real
                                       real
                                       gmx_unused *nbl,
                                       gmx_unused *nbat,
                                       gmx_unused *ic,
                                       gmx_unused *shift_vec,
                                       gmx_unused *f,
                                       gmx_unused *fshift,
                                       gmx_unused *Vvdw,
                                       gmx_unused *Vc)
#else /* CALC_ENERGIES */
void
nbnxn_kernel_ElecEw_VdwLJCombLB_F_2xnn(const nbnxn_pairlist_t
                                       const nbnxn_atomdata_t
                                       const interaction_const_t
                                       rvec
                                       real
                                       real
                                       gmx_unused *nbl,
                                       gmx_unused *nbat,
                                       gmx_unused *ic,
                                       gmx_unused *shift_vec,
                                       gmx_unused *f,
                                       gmx_unused *fshift)
#endif /* CALC_ENERGIES */
```

File Generator (3) – Idea

- First let's look at the three files included:
 - *nbnxn_kernel_simd_2xnn.h* -> defines the lookup table
 - *nbnxn_kernel_simd_2xnn_common.h* -> some SIMD utils
 - *nbnxn_kernel_simd_2xnn_outer.h* -> defines function
- In a word, gromacs puts different function in different file with different macros, and the compiler will choose which instructions should be included

Basic Workflow (1)

1. There is a call for **nbnxn_kernel_simd_2xnn**
2. **nbnxn_kernel_simd_2xnn** decides which generated function to call and find the function inside the lookup table
3. function will run and return the result

Basic Workflow(2)

- So where's our work?
 - inside **nbnxn_kernel_simd_2xnn** the kernel step is a loop contains procedure call for the generated function;
 - this loop has been wrapped with *omp parallel for*. Although, on the Xeon Host.
 - in the function body of the generated function, a lot of SIMD functions have been called;
 - however, I'm not sure whether their vector length is suitable for the Xeon Phi VPU