Pacific Northwest
NATIONAL LABORATORY

Programming MiniMD with MCL

PPoPP ‘22

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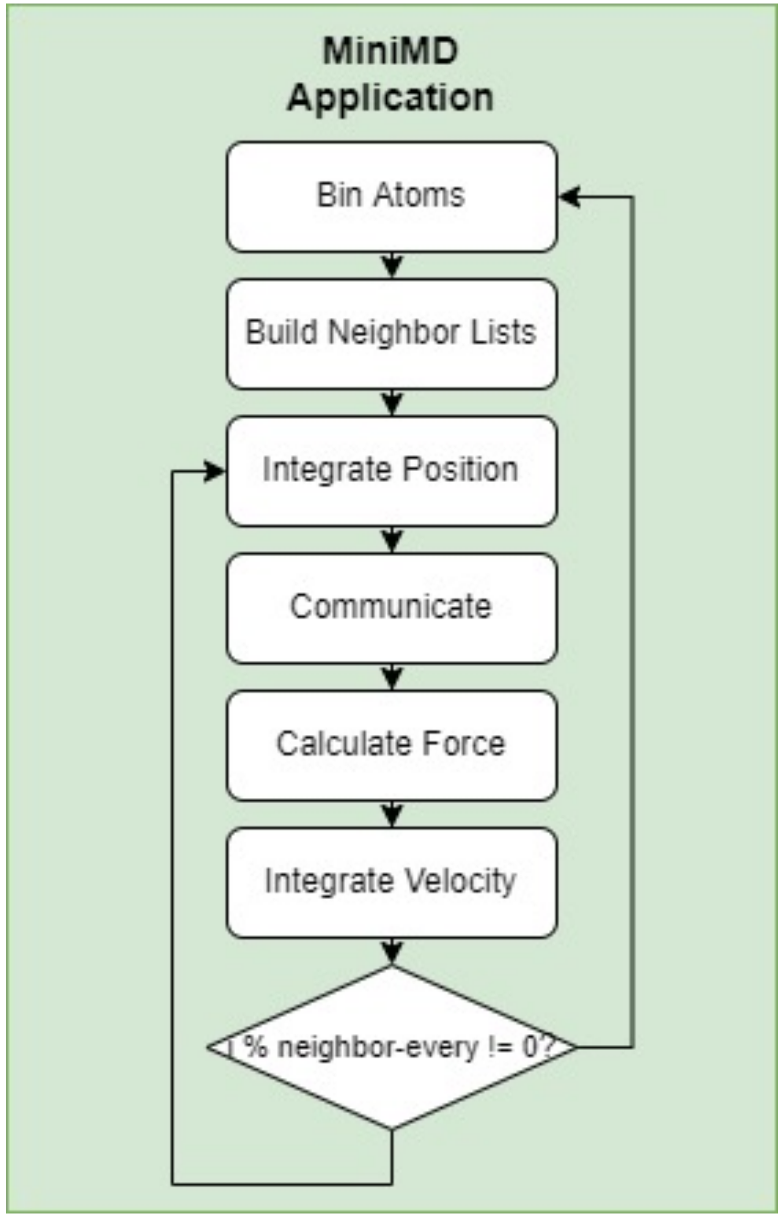
MiniMD Application Background

- Based off LAMMPS MD code (from Sandia National Lab) - https://github.com/Mantevo/miniMD
- Uses a spatial decomposition to break the problem over multiple processors (or multiple GPUs)
- Uses neighbor lists for the force calculation – reduces work, but relies on random memory accesses
- MCL currently only supports Lennard-Jones interactions for the simulation

MiniMD Structure

- Composed of 6 different kernels/tasks
- MPI - Atoms are divided into different processes -1 process per GPU
- MCL – 1 client process
  - No need for inter-process communication
- Maintain spatial decomposition of atoms - same number of tasks, same memory footprint



MiniMD Application

Bin Atoms

Build Neighbor Lists

Integrate Position

Communicate

Calculate Force

Integrate Velocity

i % neighbor-every != 0?

MiniMD-MCL

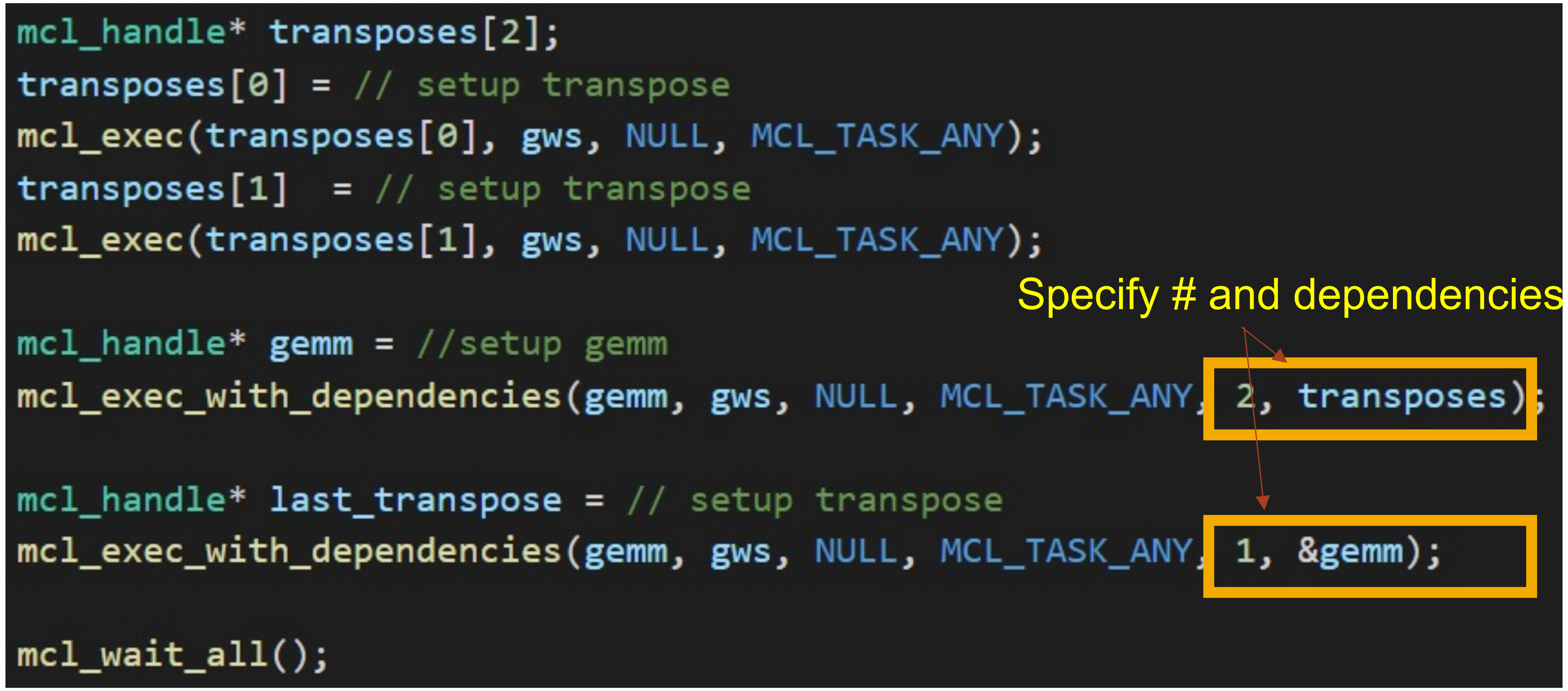
- Advantages:
  - **Kernels reused** from OpenCL
  - **Dynamic Scheduling** – GPU allocation adapts to system use
  - **Portable** –Nvidia GPUs, AMD GPUs, and GPU + Xilinx FPGA
  - **Ease of Use**
- Disadvantages:
  - **Scheduling Overhead**

Preliminaries: Resident Memory

- May need to mark certain data as “resident” to MCL
  - i.e. Multiple tasks use the same piece of data, output of one task is input to another, etc.
- Can mark these arguments with MCL_ARG_RESIDENT.
- MCL_ARG_DYNAMIC – pass data from task to task
- Scheduler manages transfers to correct device
- Allocation **could** exist till:
  - MCL_ARG_DONE flag is passed
  - mcl_unregister_buffer(void* buffer) is called
- Data my be on host, or any device based on scheduler and tasks

Preliminaries: Dependencies

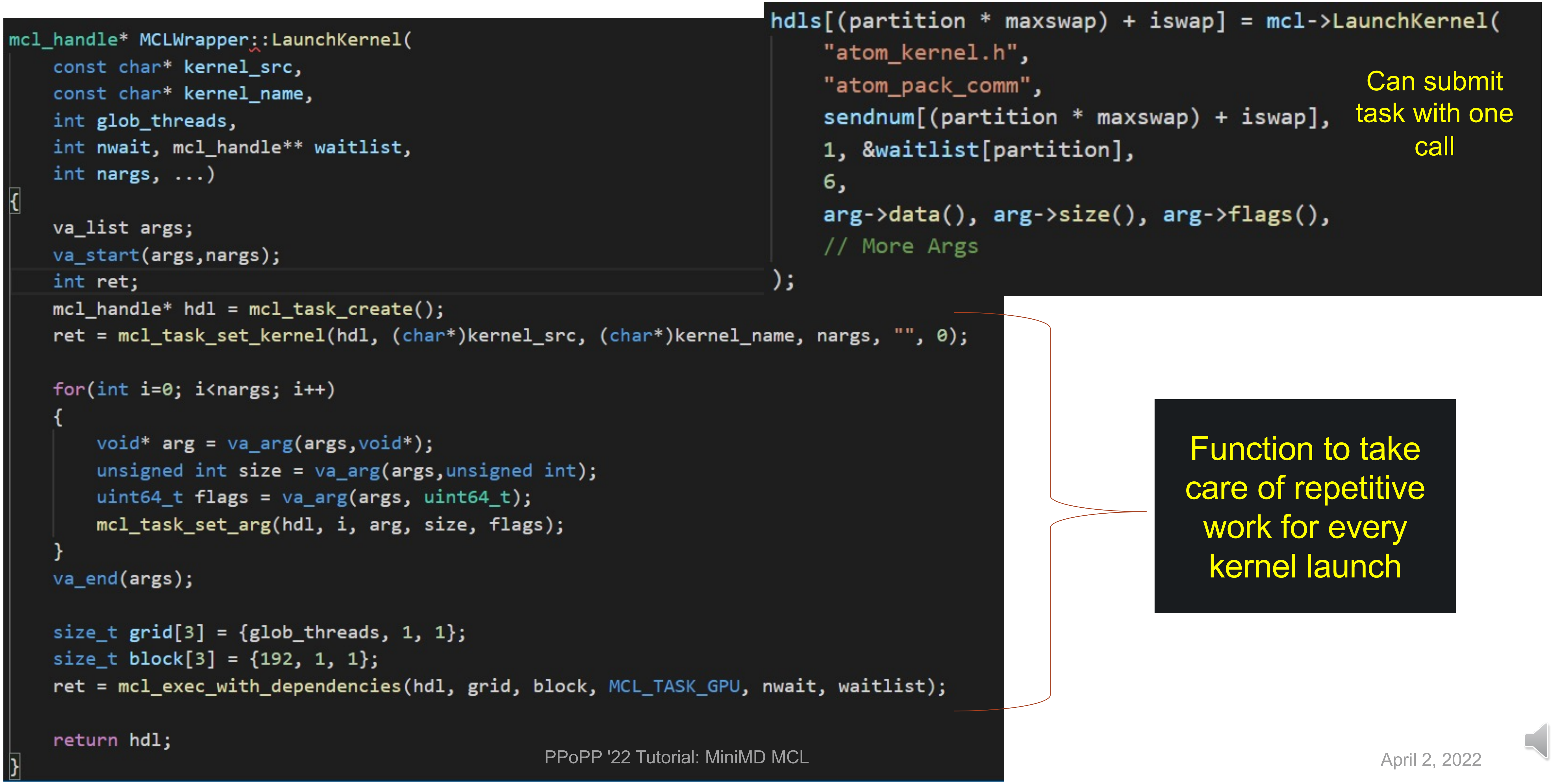
- New API
  - Asynchronous expression of dependencies
  - Quicker turn around between tasks
- Scheduling logic
  - Tasks are scheduled when all immediate dependencies are executing (but before they are finished)



```
mcl_handle* transposes[2];
transposes[0] = // setup transpose
mcl_exec(transposes[0], gws, NULL, MCL_TASK_ANY);
transposes[1]  = // setup transpose
mcl_exec(transposes[1], gws, NULL, MCL_TASK_ANY);

mcl_handle* gemm = //setup gemm
mcl_exec_with_dependencies(gemm, gws, NULL, MCL_TASK_ANY, 2, transposes);

mcl_handle* last_transpose = // setup transpose
mcl_exec_with_dependencies(gemm, gws, NULL, MCL_TASK_ANY, 1, &gemm);

mcl_wait_all();
```

Specify # and dependencies

Preliminaries: Boilerplate



```
mcl_handle* MCLWrapper::LaunchKernel(
    const char* kernel_src,
    const char* kernel_name,
    int glob_threads,
    int nwait, mcl_handle** waitlist,
    int nargs, ...)
{
    va_list args;
    va_start(args,nargs);
    int ret;
    mcl_handle* hdl = mcl_task_create();
    ret = mcl_task_set_kernel(hdl, (char*)kernel_src, (char*)kernel_name, nargs, "", 0);

    for(int i=0; i<nargs; i++)
    {
        void* arg = va_arg(args,void*);
        unsigned int size = va_arg(args,unsigned int);
        uint64_t flags = va_arg(args, uint64_t);
        mcl_task_set_arg(hdl, i, arg, size, flags);
    }
    va_end(args);

    size_t grid[3] = {glob_threads, 1, 1};
    size_t block[3] = {192, 1, 1};
    ret = mcl_exec_with_dependencies(hdl, grid, block, MCL_TASK_GPU, nwait, waitlist);

    return hdl;
}
```

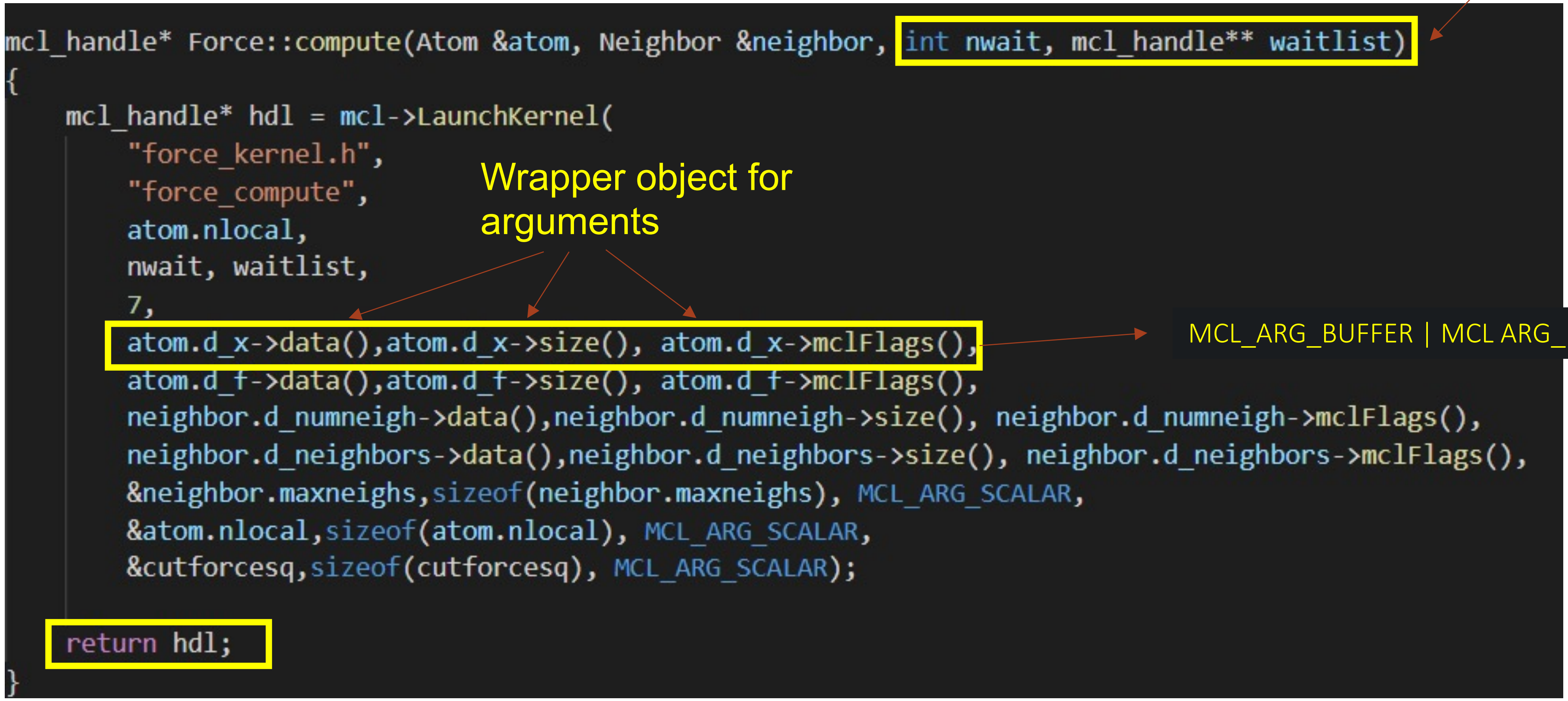
```
hdls[(partition * maxswap) + iswap] = mcl->LaunchKernel(
    "atom_kernel.h",
    "atom_pack_comm",
    sendnum[(partition * maxswap) + iswap],
    1, &waitlist[partition],
    6,
    arg->data(), arg->size(), arg->flags(),
    // More Args
);
```

Can submit task with one call

Function to take care of repetitive work for every kernel launch

Example: Force

Pass around waitlist to manage dependencies

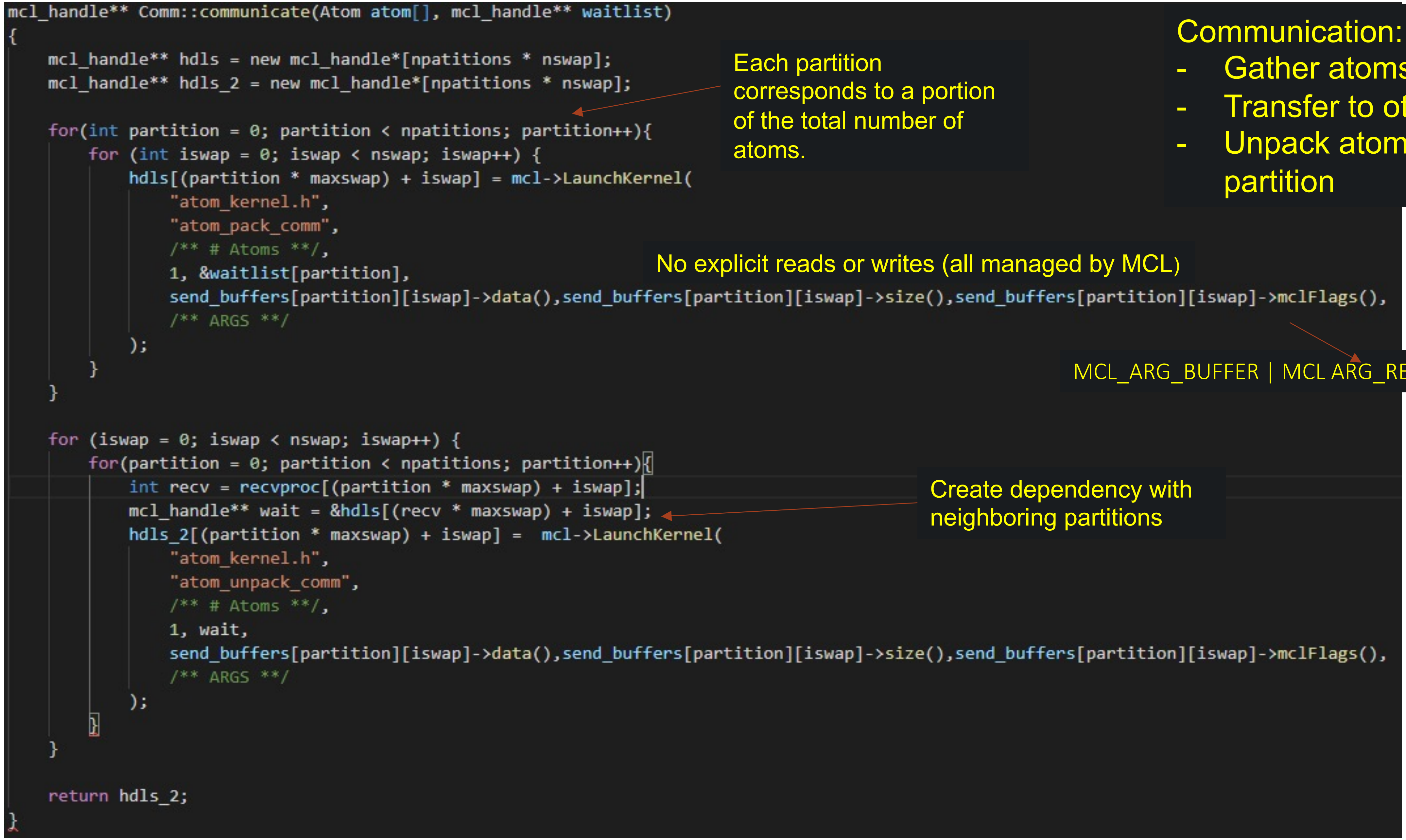


```
mcl_handle* Force::compute(Atom &atom, Neighbor &neighbor, int nwait, mcl_handle** waitlist)
{
    mcl_handle* hdl = mcl->LaunchKernel(
        "force_kernel.h",
        "force_compute",
        atom.nlocal,
        nwait, waitlist,
        7,
        atom.d_x->data(),atom.d_x->size(), atom.d_x->mclFlags(),
        atom.d_f->data(),atom.d_f->size(), atom.d_f->mclFlags(),
        neighbor.d_numneigh->data(),neighbor.d_numneigh->size(), neighbor.d_numneigh->mclFlags(),
        neighbor.d_neighbors->data(),neighbor.d_neighbors->size(), neighbor.d_neighbors->mclFlags(),
        &neighbor.maxneighs,sizeof(neighbor.maxneighs), MCL_ARG_SCALAR,
        &atom.nlocal,sizeof(atom.nlocal), MCL_ARG_SCALAR,
        &cutforcesq,sizeof(cutforcesq), MCL_ARG_SCALAR);

    return hdl;
}
```

Wrapper object for arguments

MCL_ARG_BUFFER | MCL ARG_RESIDENT | MCL_ARG_DYNAMIC

Example: Communication



```
mcl_handle** Comm::communicate(Atom atom[], mcl_handle** waitlist)
{
    mcl_handle** hdls = new mcl_handle*[npatitions * nswap];
    mcl_handle** hdls_2 = new mcl_handle*[npatitions * nswap];

    for(int partition = 0; partition < npatitions; partition++){
        for (int iswap = 0; iswap < nswap; iswap++) {
            hdls[(partition * maxswap) + iswap] = mcl->LaunchKernel(
                "atom_kernel.h",
                "atom_pack_comm",
                /** # Atoms **/,
                1, &waitlist[partition],
                send_buffers[partition][iswap]->data(),send_buffers[partition][iswap]->size(),send_buffers[partition][iswap]->mclFlags(),
                /** ARGS **/
            );
        }
    }

    for (iswap = 0; iswap < nswap; iswap++) {
        for(partition = 0; partition < npatitions; partition++){
            int recv = recvproc[(partition * maxswap) + iswap];
            mcl_handle** wait = &hdls[(recv * maxswap) + iswap];
            hdls_2[(partition * maxswap) + iswap] =  mcl->LaunchKernel(
                "atom_kernel.h",
                "atom_unpack_comm",
                /** # Atoms **/,
                1, wait,
                send_buffers[partition][iswap]->data(),send_buffers[partition][iswap]->size(),send_buffers[partition][iswap]->mclFlags(),
                /** ARGS **/
            );
        }
    }

    return hdls_2;
}
```

Communication:
- Gather atoms on boundary of partition
- Transfer to other partition
- Unpack atoms to proper place in partition

Each partition corresponds to a portion of the total number of atoms.

No explicit reads or writes (all managed by MCL)

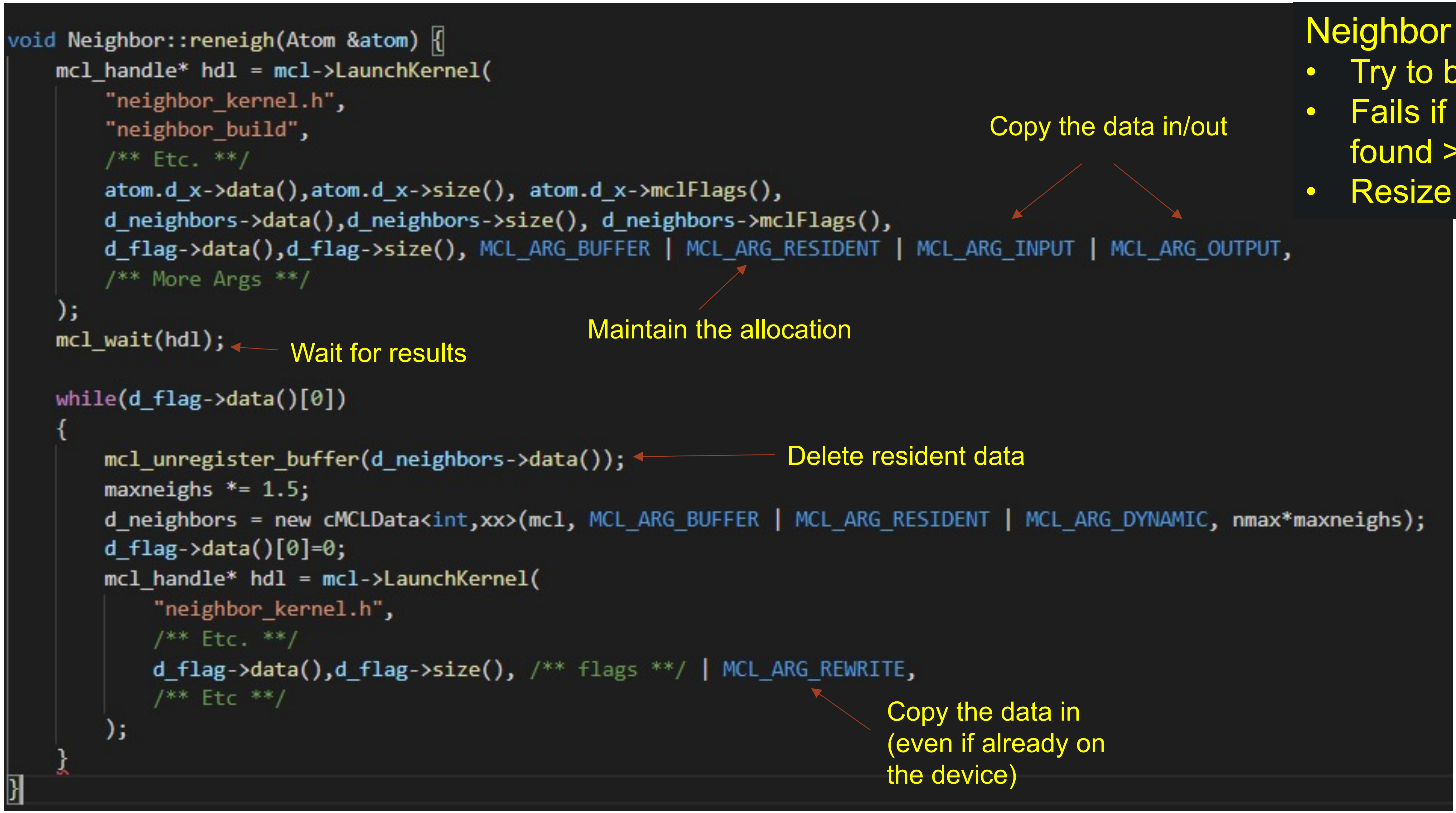
MCL_ARG_BUFFER | MCL ARG_RESIDENT | MCL_ARG_DYNAMIC

Create dependency with neighboring partitions

Example: Neighboring

Neighbor Build:

- Try to build neighbor lists
- Fails if num neighbors found > max neighbors
- Resize and retry on failure



```
void Neighbor::reneigh(Atom &atom) {
    mcl_handle* hdl = mcl->LaunchKernel(
        "neighbor_kernel.h",
        "neighbor_build",
        /** Etc. **/
        atom.d_x->data(),atom.d_x->size(), atom.d_x->mclFlags(),
        d_neighbors->data(),d_neighbors->size(), d_neighbors->mclFlags(),
        d_flag->data(),d_flag->size(), MCL_ARG_BUFFER | MCL_ARG_RESIDENT | MCL_ARG_INPUT | MCL_ARG_OUTPUT,
        /** More Args **/
    );
    mcl_wait(hdl);

    while(d_flag->data()[0])
    {
        mcl_unregister_buffer(d_neighbors->data());
        maxneighs *= 1.5;
        d_neighbors = new cMCLData<int,xx>(mcl, MCL_ARG_BUFFER | MCL_ARG_RESIDENT | MCL_ARG_DYNAMIC, nmax*maxneighs);
        d_flag->data()[0]=0;
        mcl_handle* hdl = mcl->LaunchKernel(
            "neighbor_kernel.h",
            /** Etc. **/
            d_flag->data(),d_flag->size(), /** flags **/ | MCL_ARG_REWRITE,
            /** Etc **/
        );
    }
}
```

Copy the data in/out

Maintain the allocation

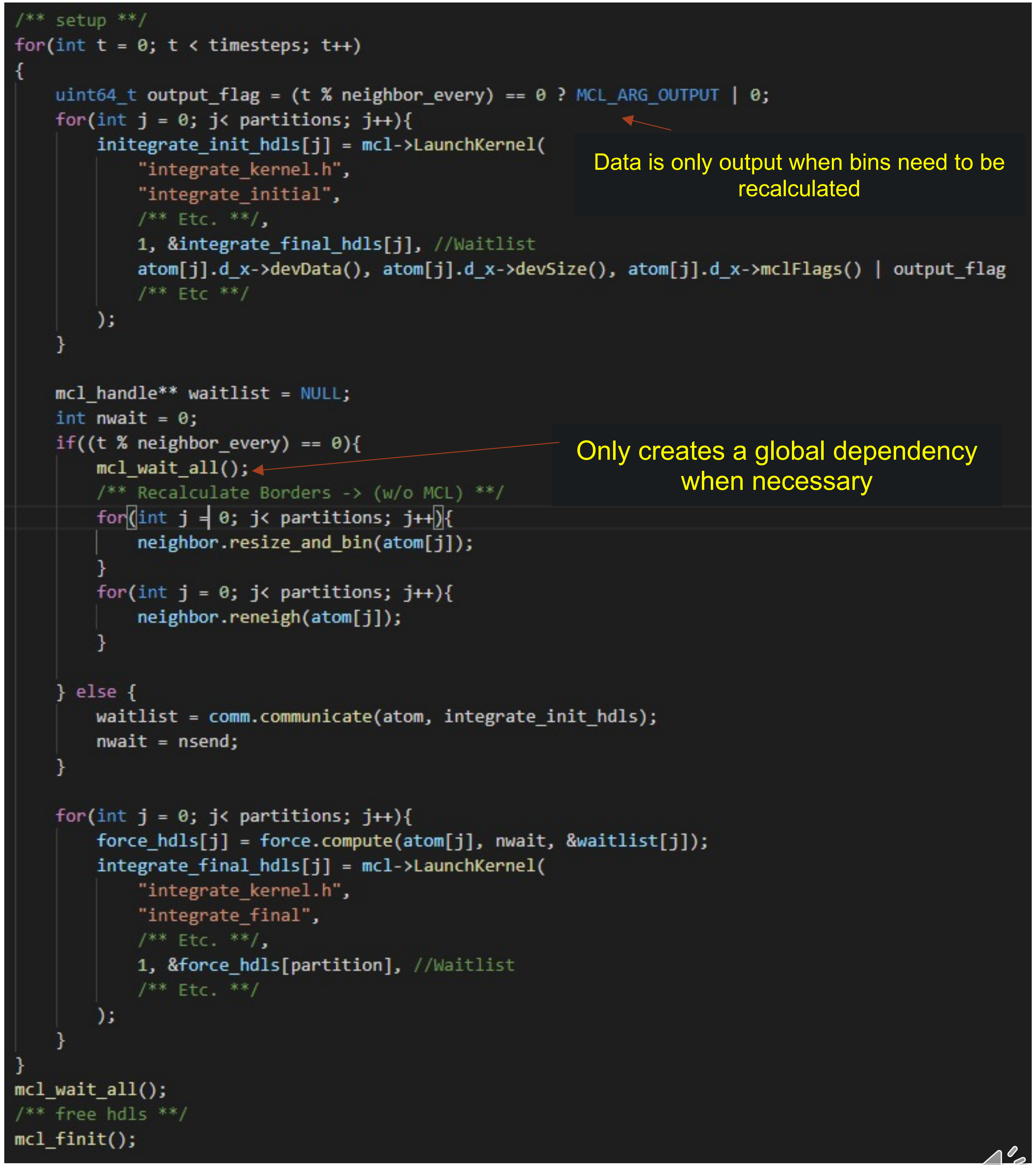
Wait for results

Delete resident data

Copy the data in (even if already on the device)

Example: Integrate

Integrate:
- Step through time calculating position, force, and velocity
- Launch calculations for all partitions asynchronously
- Every ~20 timesteps, recalculate the partitions of the atoms

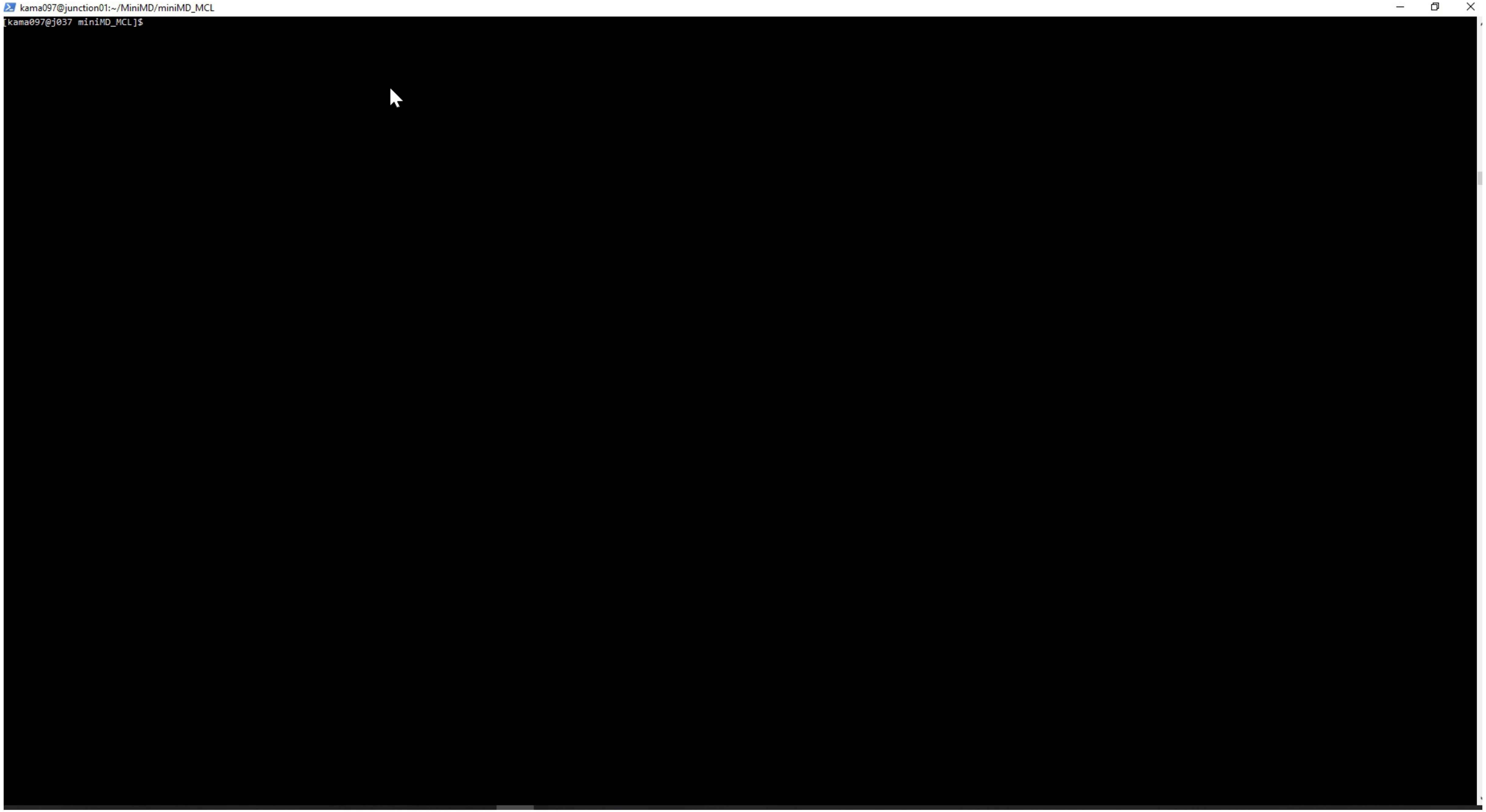


```
/** setup **/
for(int t = 0; t < timesteps; t++)
{
    uint64_t output_flag = (t % neighbor_every) == 0 ? MCL_ARG_OUTPUT | 0;
    for(int j = 0; j< partitions; j++){
        initegrate_init_hdls[j] = mcl->LaunchKernel(
            "integrate_kernel.h",
            "integrate_initial",
            /** Etc. **/,
            1, &integrate_final_hdls[j], //Waitlist
            atom[j].d_x->devData(), atom[j].d_x->devSize(), atom[j].d_x->mclFlags() | output_flag
            /** Etc **/
        );
    }

    mcl_handle** waitlist = NULL;
    int nwait = 0;
    if((t % neighbor_every) == 0){
        mcl_wait_all();
        /** Recalculate Borders -> (w/o MCL) **/
        for(int j = 0; j< partitions; j++){
            neighbor.resize_and_bin(atom[j]);
        }
        for(int j = 0; j< partitions; j++){
            neighbor.reneigh(atom[j]);
        }

    } else {
        waitlist = comm.communicate(atom, integrate_init_hdls);
        nwait = nsend;
    }

    for(int j = 0; j< partitions; j++){
        force_hdls[j] = force.compute(atom[j], nwait, &waitlist[j]);
        integrate_final_hdls[j] = mcl->LaunchKernel(
            "integrate_kernel.h",
            "integrate_final",
            /** Etc. **/,
            1, &force_hdls[partition], //Waitlist
            /** Etc. **/
        );
    }
}
mcl_wait_all();
/** free hdls **/
mcl_finit();
```

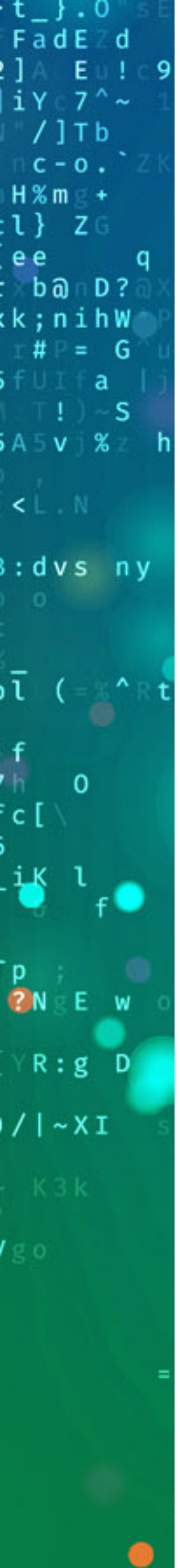
Data is only output when bins need to be recalculated

Only creates a global dependency when necessary

Demo



```
[kama097@j037 miniMD_MCL]$
```



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Thank you