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Code Handover

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Table 1: Files for Langevin simulation and check solver-correctness.

Filename	Description
<code>Langevin.cpp</code>	Contains setup and simulation loop
<code>LangevinParticles.hpp</code>	Langevin related functionality / solvers (derives from <code>ChargedParticles.hpp</code>)
<code>LangevinHelpers.hpp</code>	I.C.'s generators / Field manipulations and error computation functions used in <code>TestLangevinPotentials.cpp</code>
<code>LangevinIO.hpp</code>	Dumping functions for VTK and CSV files
<code>TestLangevinPotentials.cpp</code>	File testing error convergence for multiple gridsizes

Execute Solver and Convergence Tests

- Contain default arguments mentioned in Appendix I of the report
- `local_*.sh` scripts have adapted parameters due to hardware constraints
- The programs cannot run with multiple MPI ranks
- All scripts take a cmdline arg. defining where the data should be stored (that is also appended by a timestamp)

Table 2: How to run the compiled binaries.

Filename	Description
<code>./local_langevin.sh</code>	Run Langevin solver locally
<code>./local_testPotentials.sh</code>	Run convergence tests locally
<code>sbatch slurm_langevin.sh</code>	Run Langevin solver on gmerlin
<code>sbatch slurm_gpu_langevin.sh</code>	Run Langevin solver on gmerlin
<code>sbatch slurm_testPotentials.sh</code>	Run convergence tests on merlin

- Jupyter notebooks with README.md are uploaded to [Gitlab](#)
- Notebooks to explore / plot / analyze data generated by the Langevin simulation
- Contains requirements.txt to generate Python environment with all needed packages

- After merging changes compiling on CUDA does not work
- OpenMPI runtime error (Kokkos initialization)
- CUDA compilation error: `nvcc_wrapper` does not accept standard flags `std=c2a` since partial standard flags and standards after C17 are not supported. `nvcc_wrapper` will use `std=c14` instead. It is undefined behavior to use this flag. This should only be occurring during CMake configuration.

```
000001104J  
(_ZN6Kokkos4Impl23throw_runtime_exceptionERKNSt7__cxx1112basic_stringIcSt11char_traitsIcESa1cEEE+0x31>  
(_ZN6Kokkos4Impl28parse_command_line_argumentsER1PPcRNS_22InitializationSettingsE+0x12f3)[0x974ba3]  
(_ZN6Kokkos10initializeERiPPc+0x4d)[0x9752ed]  
(_ZN4ippl10initializeER1PPcP19mpi_communicator_t+0x885)[0x964018]  
(main+0x3d)[0x7be3c4]
```

Figure 1: OpenMPI runtime error.