CUDA and ROCm GPU Ionic Models: Raw Performance and Energy Performance

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EuroHPC Joint Undertaking

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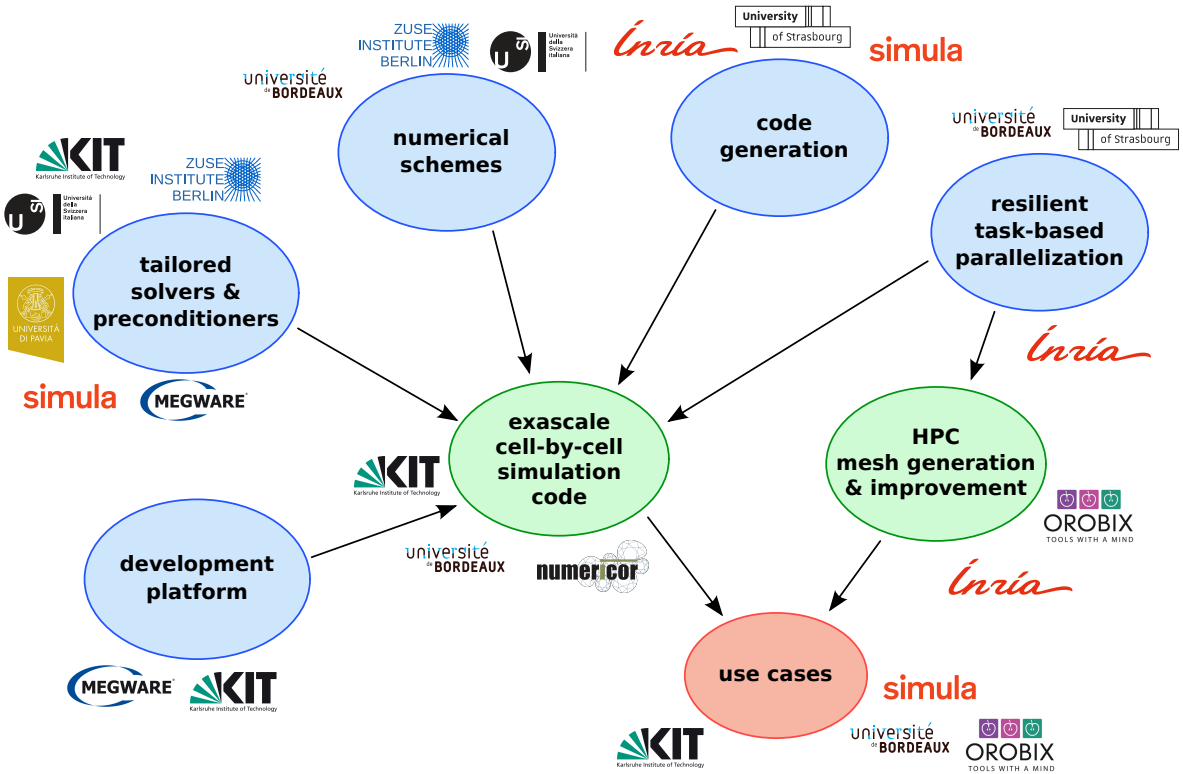
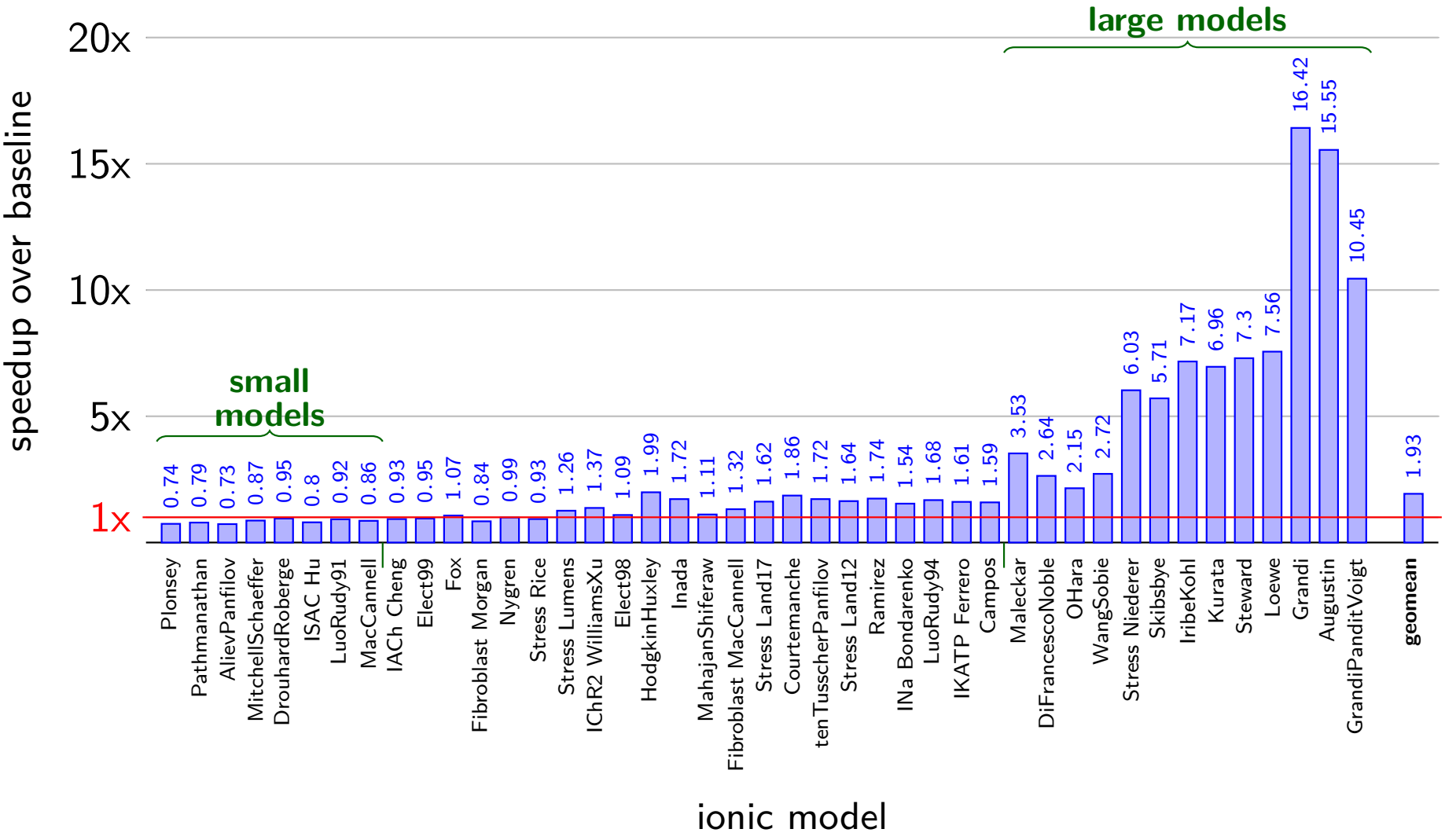
WP6 - Code Generation for Ionic Models



Outline

Performance: AVX-512; **32 Cores**; Cells - 8192



Why MLIR?

- parallelization: OpenMP is easy (and done) the loop is parallel
- loop optimization: standard techniques, polyhedral and many others
- vectorization:
  - $\rightarrow$ need to do it manually or at the compiler level

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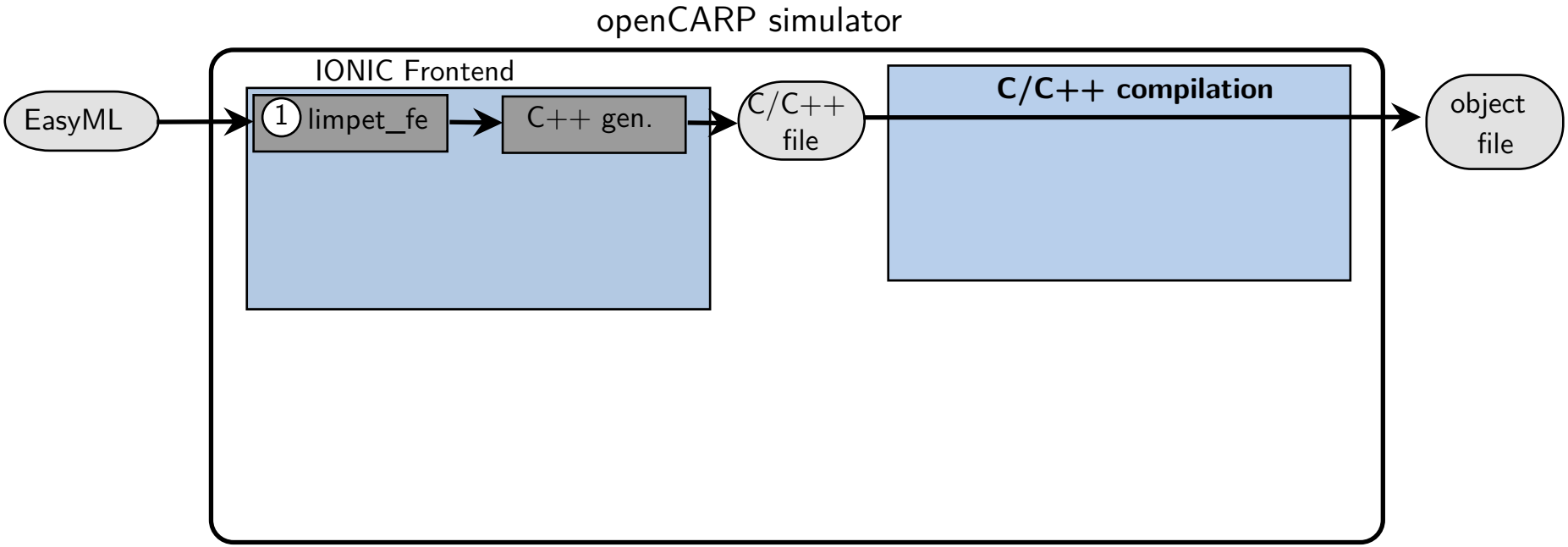
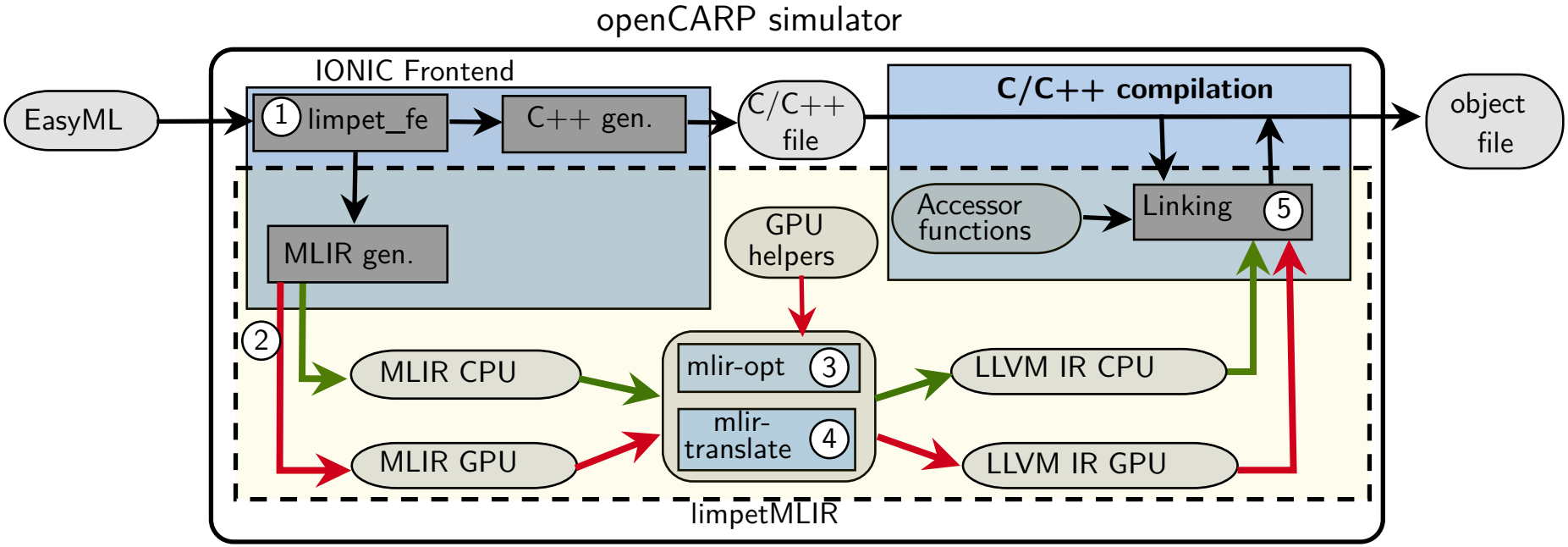
→ using an existing compiler infrastructure - **MLIR**
to benefit from generality, other optimizations
and automatic code generation passes

Outline

openCARP - Compilation Flow

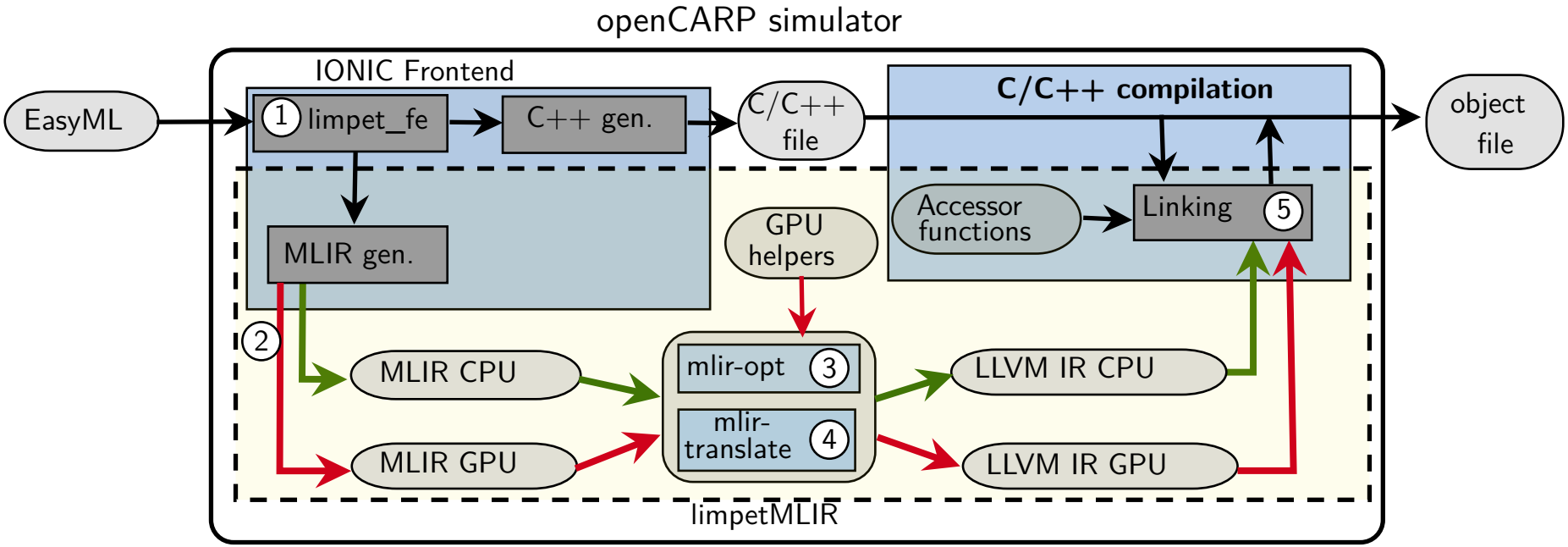


limpetMLIR: Our Proposed Compilation Flow



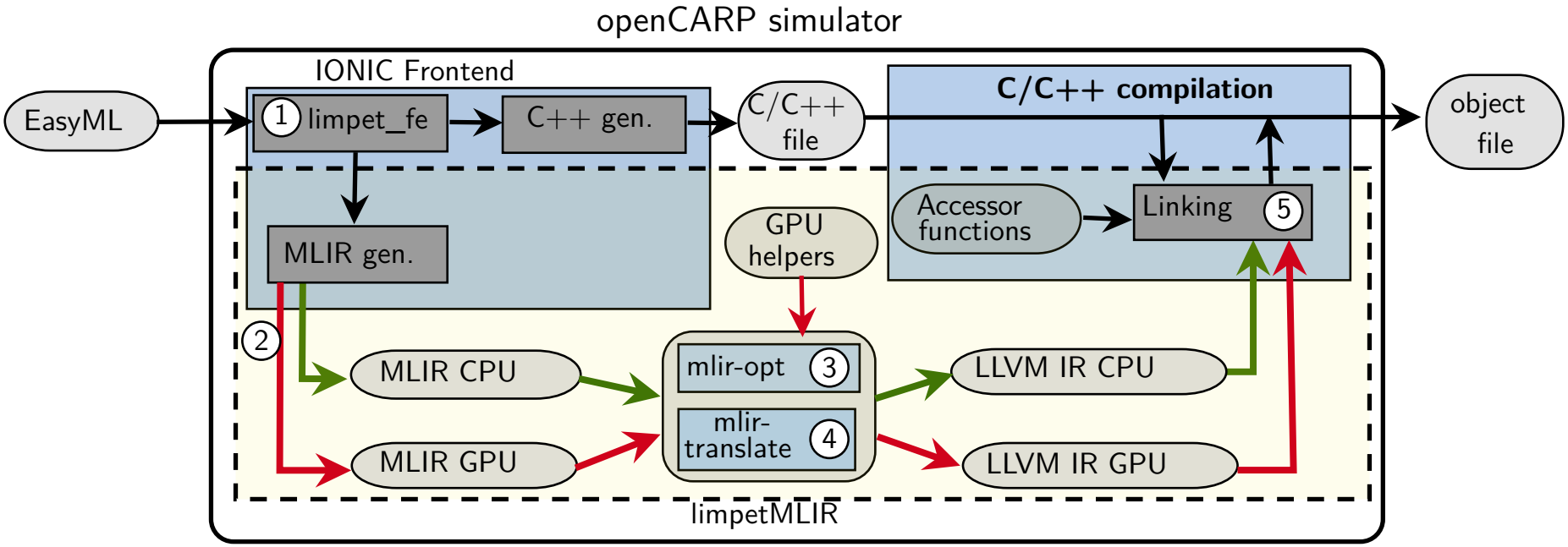
1 - From EasyML DSL the `limpet_fe` python script generates an AST, which serves as a common entry point for baseline openCARP and limpetMLIR.

limpetMLIR: Our Proposed Compilation Flow



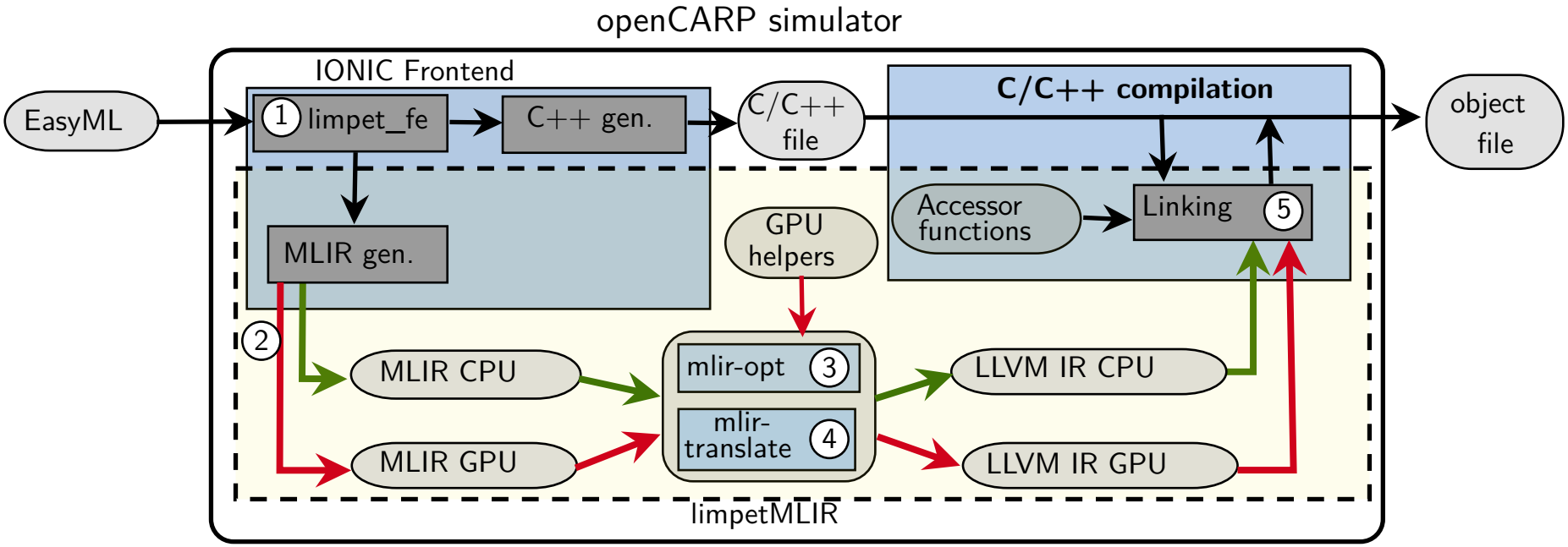
2 - Using python bindings, our limpetMLIR emits MLIR code for compute intensive kernel using `scf`, `arith`, `math` and `memref` dialects.
- Choose type `vector<?xf64>` for vectorized CPU; and `f64` for GPU.

limpetMLIR: Our Proposed Compilation Flow



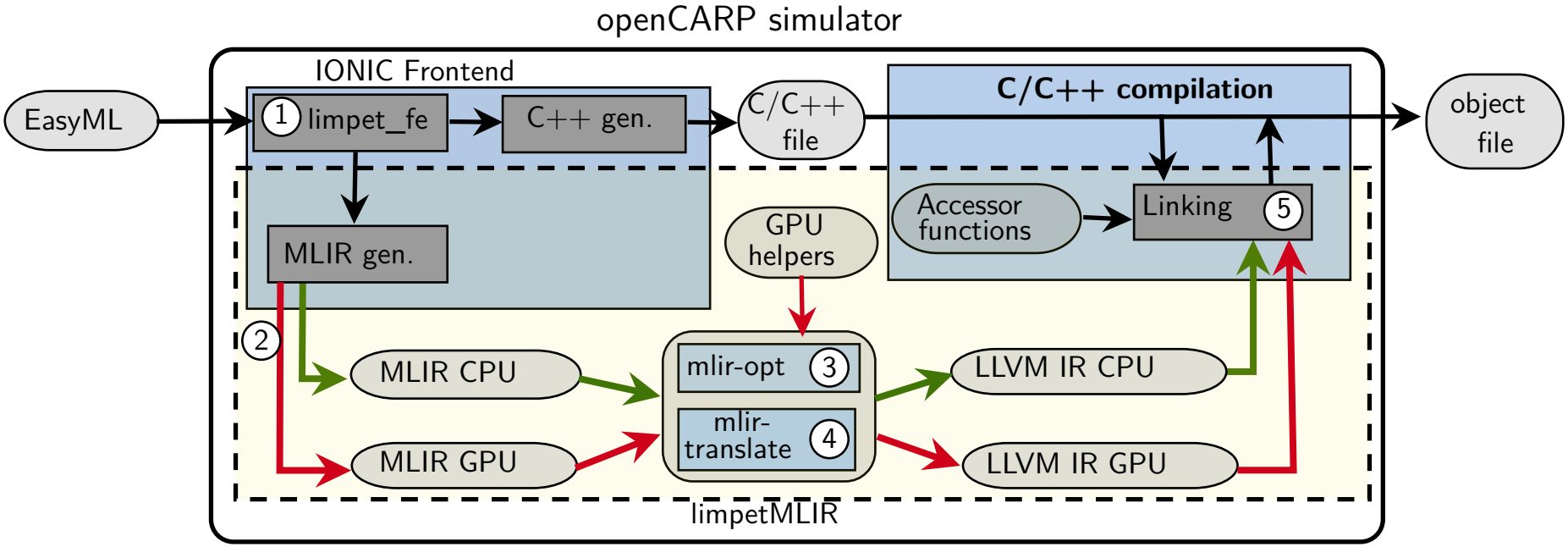
3 - MLIR lowering pass. For GPU the MLIR code can be lowered to either `nvvm` (the Nvidia CUDA IR) or `rocdl` (the AMD ROCm IR).

limpetMLIR: Our Proposed Compilation Flow



4 - MLIR translator pass converts the final MLIR code to LLVM IR (either CPU or GPU).

limpetMLIR: Our Proposed Compilation Flow



5 - Last is the linking phase, where c/c++ and LLVM IR (either CPU or GPU) are linked together into an object file.

Code generation

- Methods for temporal discretization - Euler, Runge-kutta 2 and 4, Rush-Iarsen, Sundnes, Markov, and Rosenbrock
- *GPU helper* functions $\Rightarrow$ for LUT and Rosenbrock external function calls.
- Memory management for GPUs
  - Unified memory model for CUDA (Nvidia),
  - Manual memory allocations for ROCm (AMD),
  - `/bin/bench` executable.

Outline

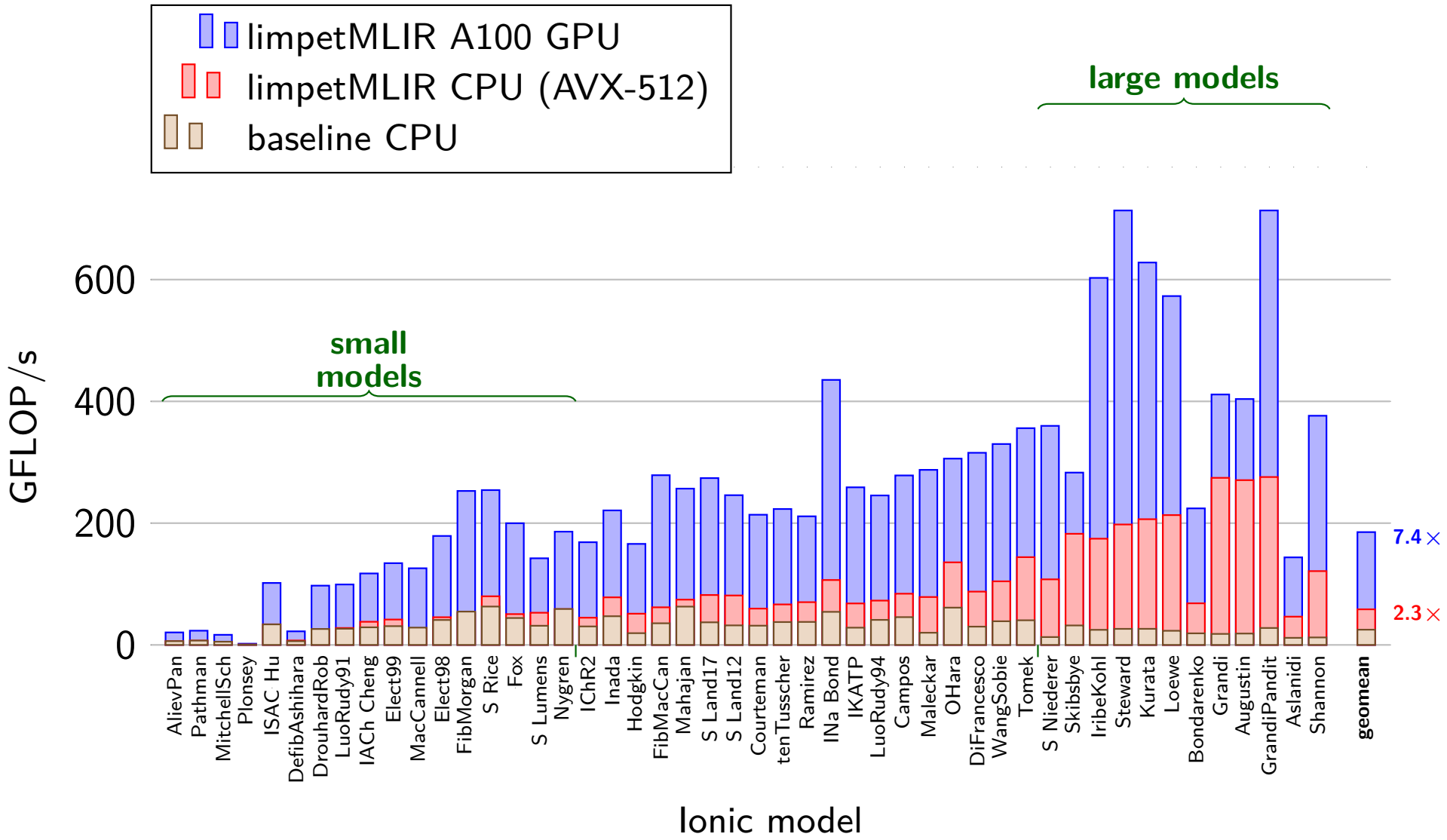
Results

- limpetMLIR implemented on top of openCARP (git master branch) using the LLVM infrastructure from trunk (version 15.0.x)
- try it with the following cmake options available at: `git.opencarp.org/openCARP/openCARP/-/blob/master/docs/BUILD_WITH_MLIR.md`
- or with the following docker file + image available at: `https://seafile.unistra.fr/f/608712e4bee94ea2a709/?dl=1`

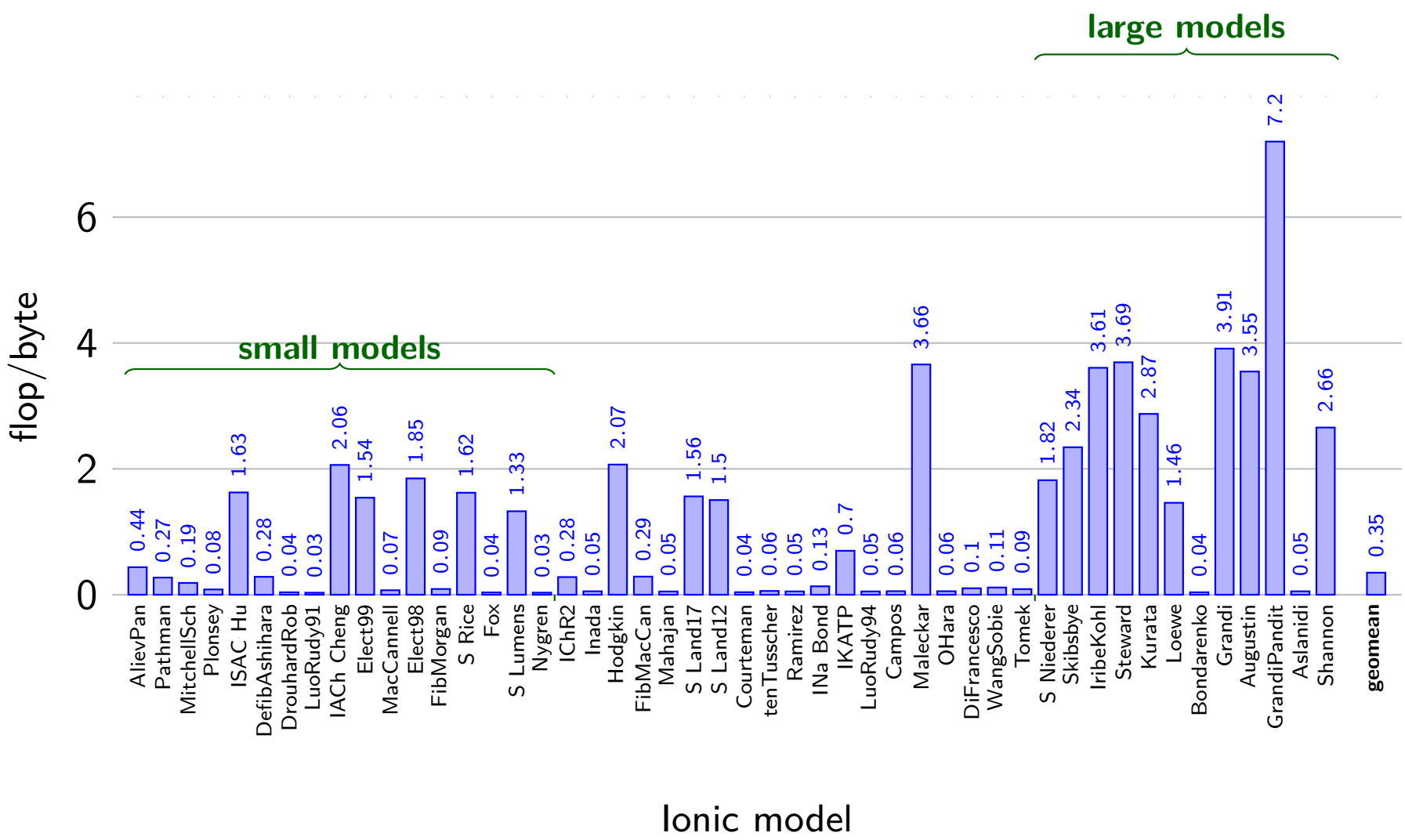
Performance evaluation

- Evaluated with 48 ionic models available in openCARP
- benchmark running the ionic model alone (`bin/bench`);
  - cells = 819,200
  - timestamp = 100
  - step = 0.01 (10,000 computation steps)
- CPU: a 2x 18-core Cascade Lake Intel Xeon Gold 6240.
- GPU:
  - an A100 Nvidia GPU (9,700 GFLOP/s peak perf. on `double`)
  - an MI50 AMD GPU (6,600 GFLOP/s peak perf. on `double`)

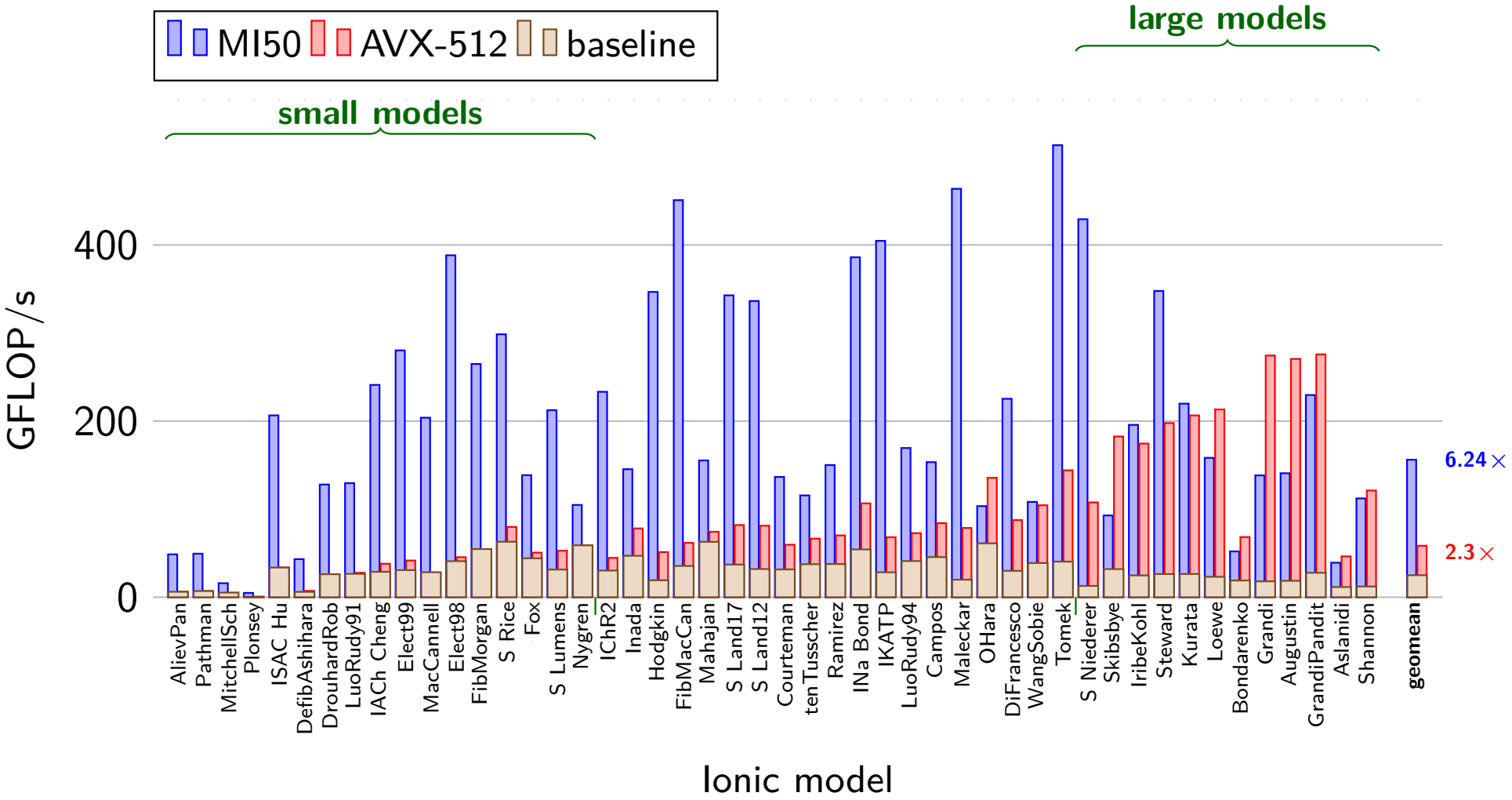
GFLOP/s performance - Nvidia A100



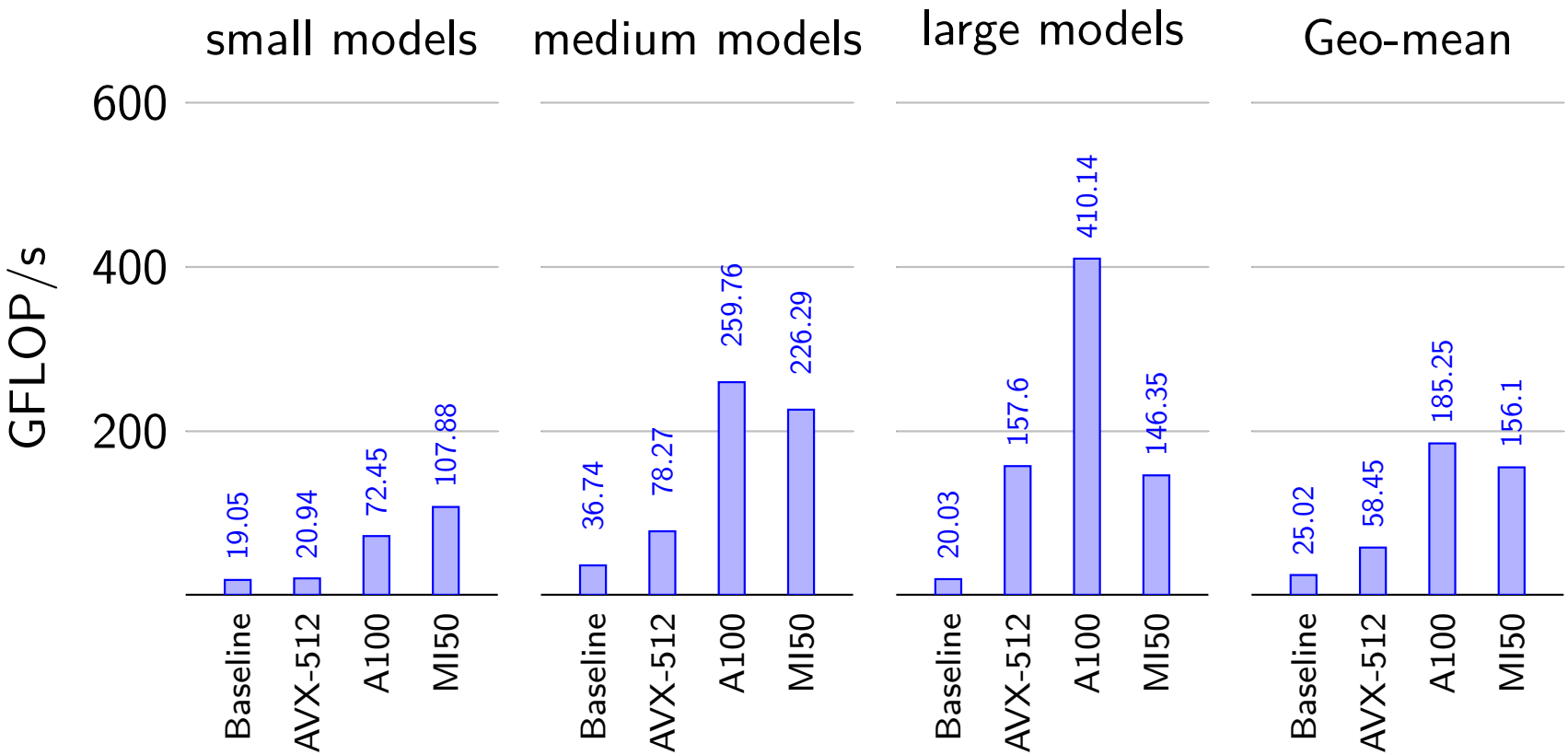
Compute-intensity of ionic models



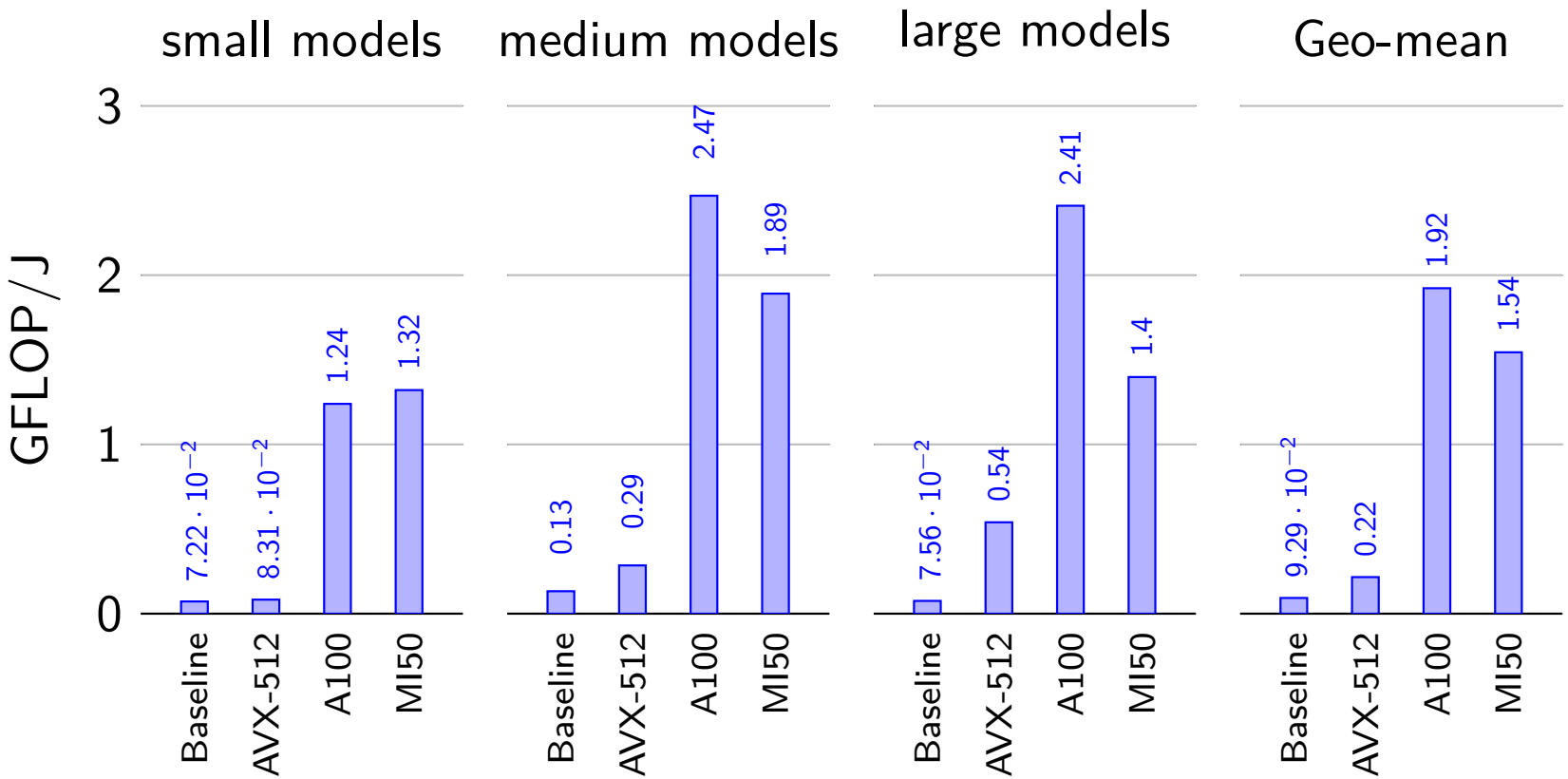
GFLOP/s performance - AMD MI50



GFLOPS/s comparision



GFLOP/J energy efficiency comparision



Outline

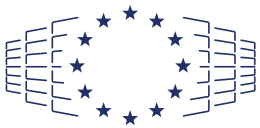
Conclusion

- ✓ GPU code generation (CUDA & ROCm)
- very good performance
  - A100: 7.40× vs baseline and 3.17× vs AVX-512
  - MI50: 6.24× vs baseline and 2.67× vs AVX-512
- very good energy efficiency
  - A100: 20.67× vs baseline and 8.73× vs AVX-512
  - MI50: 16.58× vs baseline and 7× vs AVX-512

Future interest of work:

- integrate with the solver to avoid memory transfers
- further optimization of the generated code
  (LUTs as splines, NN, Rosenbrock, FP approximations, ...)

Thank you!



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