LLVM AMDGPU for High Performance Computing: are we competitive yet?

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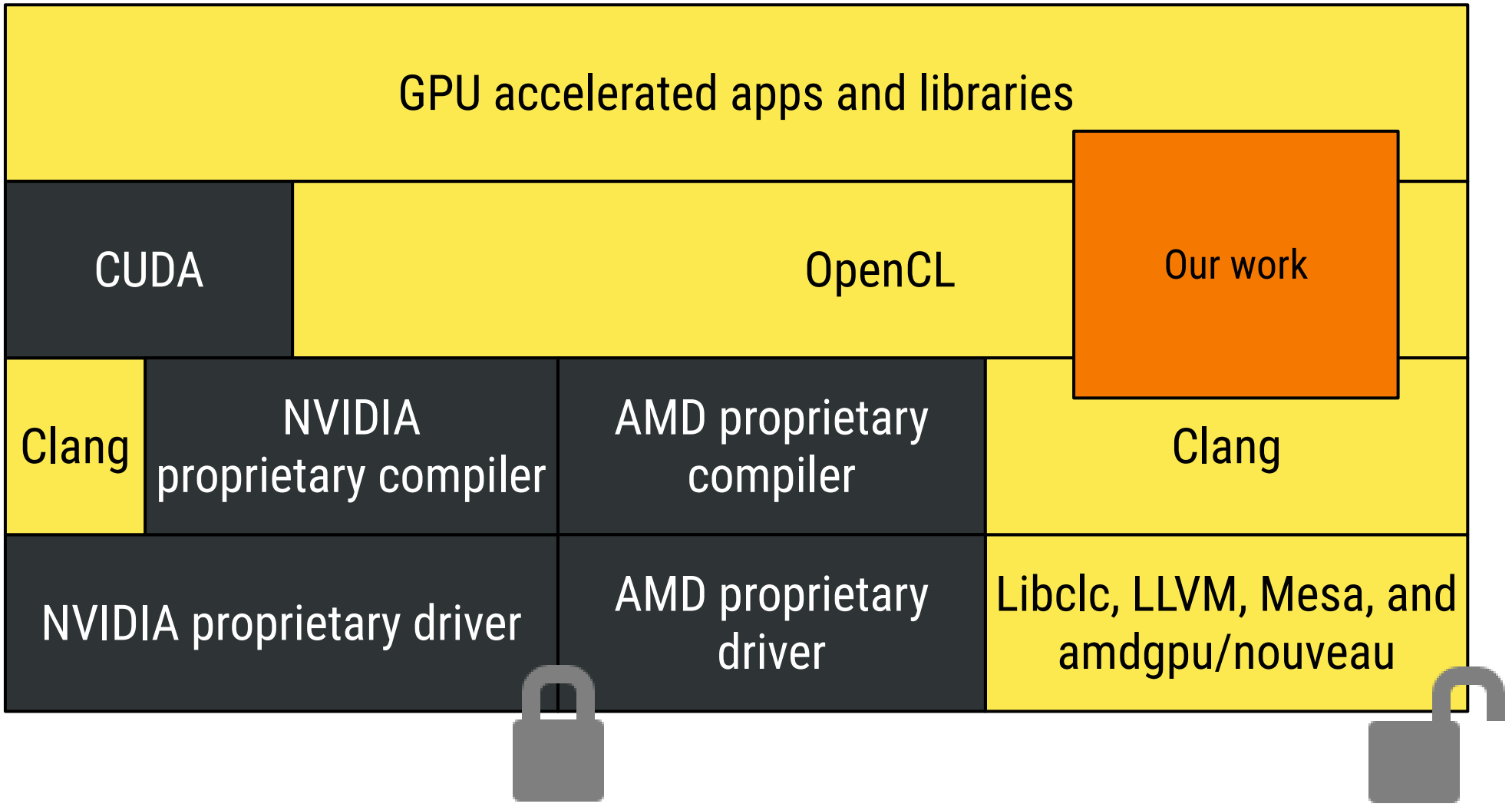
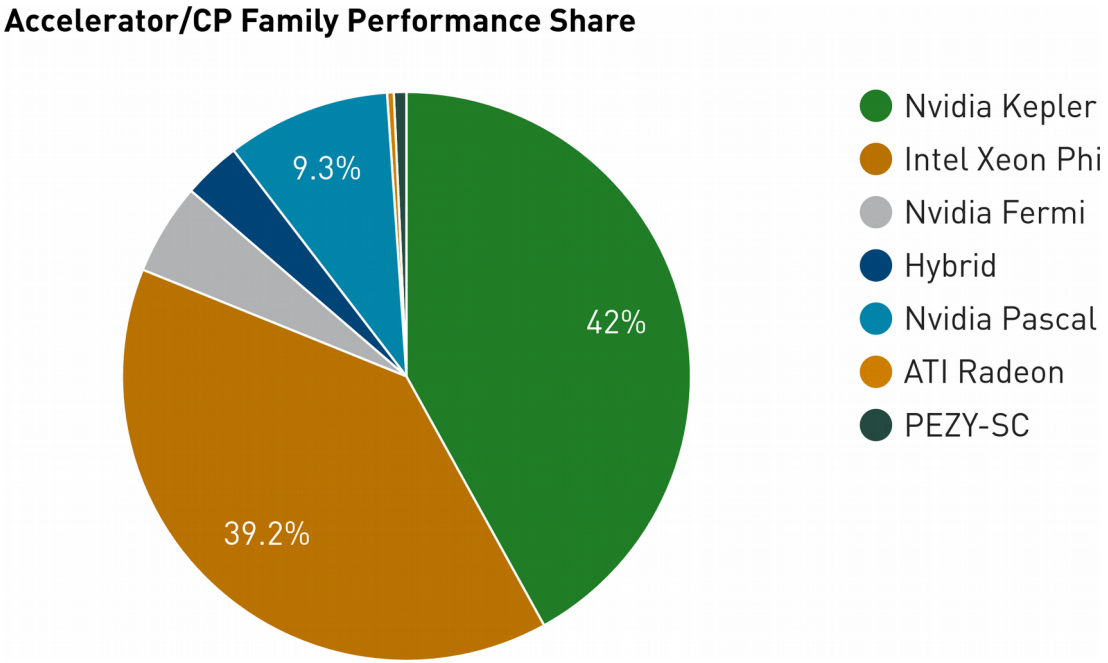
Layers of GPU computing



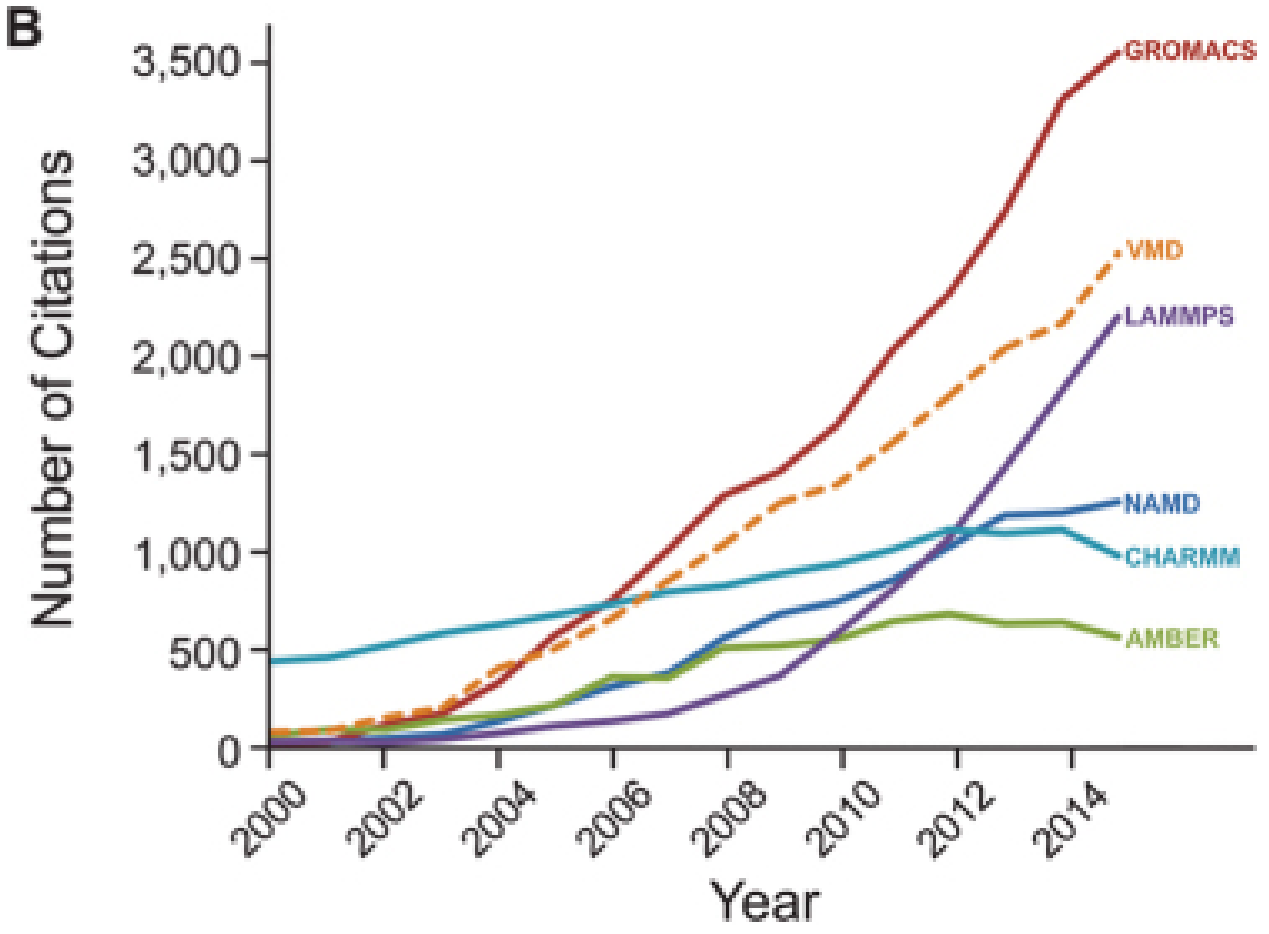
State of the art: CUDA and OpenCL

- CUDA
  - 338 applications listed at NVIDIA's website
  - Over 50% market share in Top 500 (Nov 2016)



- OpenCL
  - ~70 applications listed on Wikipedia
    - ~30 in Scientific computing category
    - Couple of benchmarks and toys

OpenCL applications



- Image taken from: Ribeiro, João V., et al. "QwikMD—Integrative Molecular Dynamics Toolkit for Novices and Experts." *Scientific reports* 6 (2016).
- Focus on **GROMACS**, **LAMMPS**, OpenMM, ASL

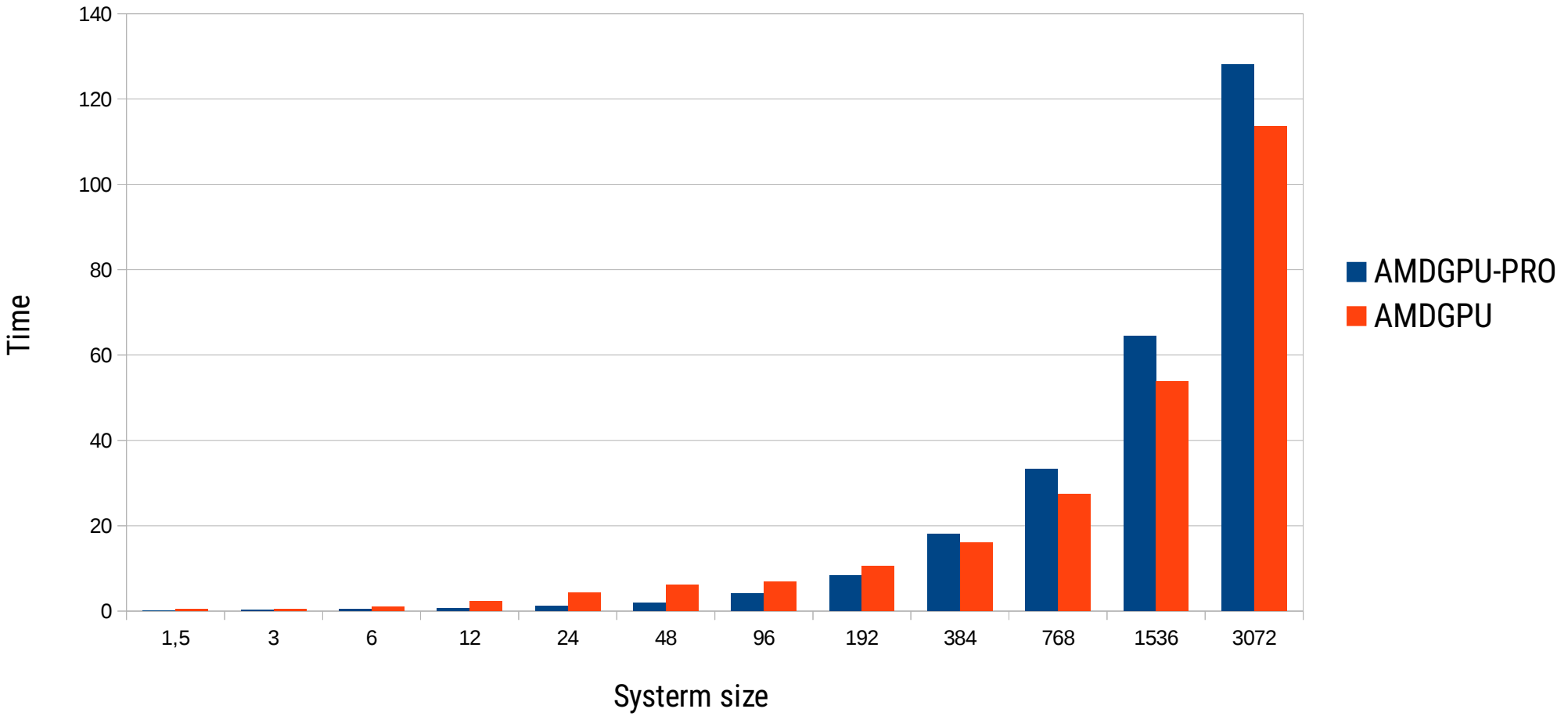
Running open source OpenCL stack on Radeon/FirePro/FireStream

- AMD's proprietary OpenCL driver and compiler
  - GPUs released 2012 or later
  - Will be open sourced soon™
- **Mesa/LLVM**
  - AMD GPUs released 2009 or later
  - Open source from the beginning™

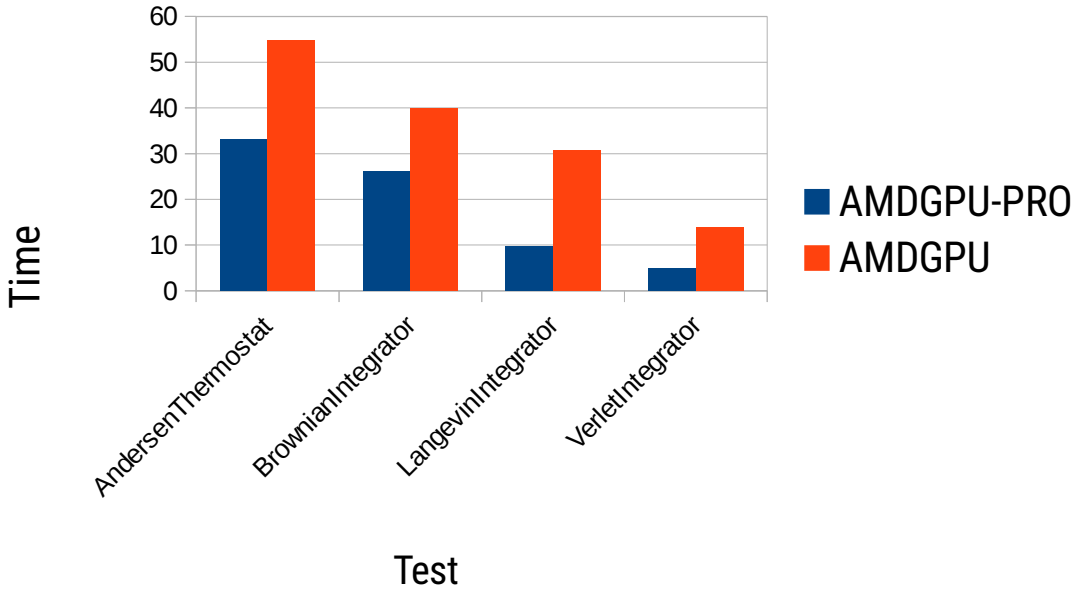
Our work

- **No changes or minor changes in apps/libs**
- Improvements to LLVM, Clang, libclc, Mesa
  - Missing math functions, OpenCL 1.2 API calls
  - Bug fixes

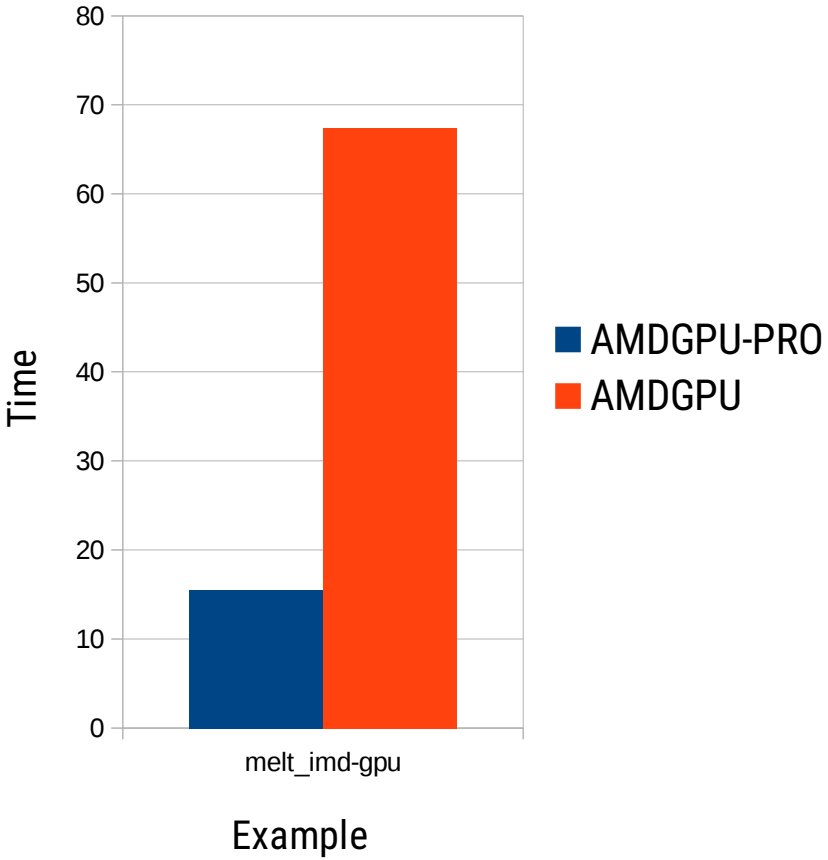
GROMACS OpenCL kernel execution time



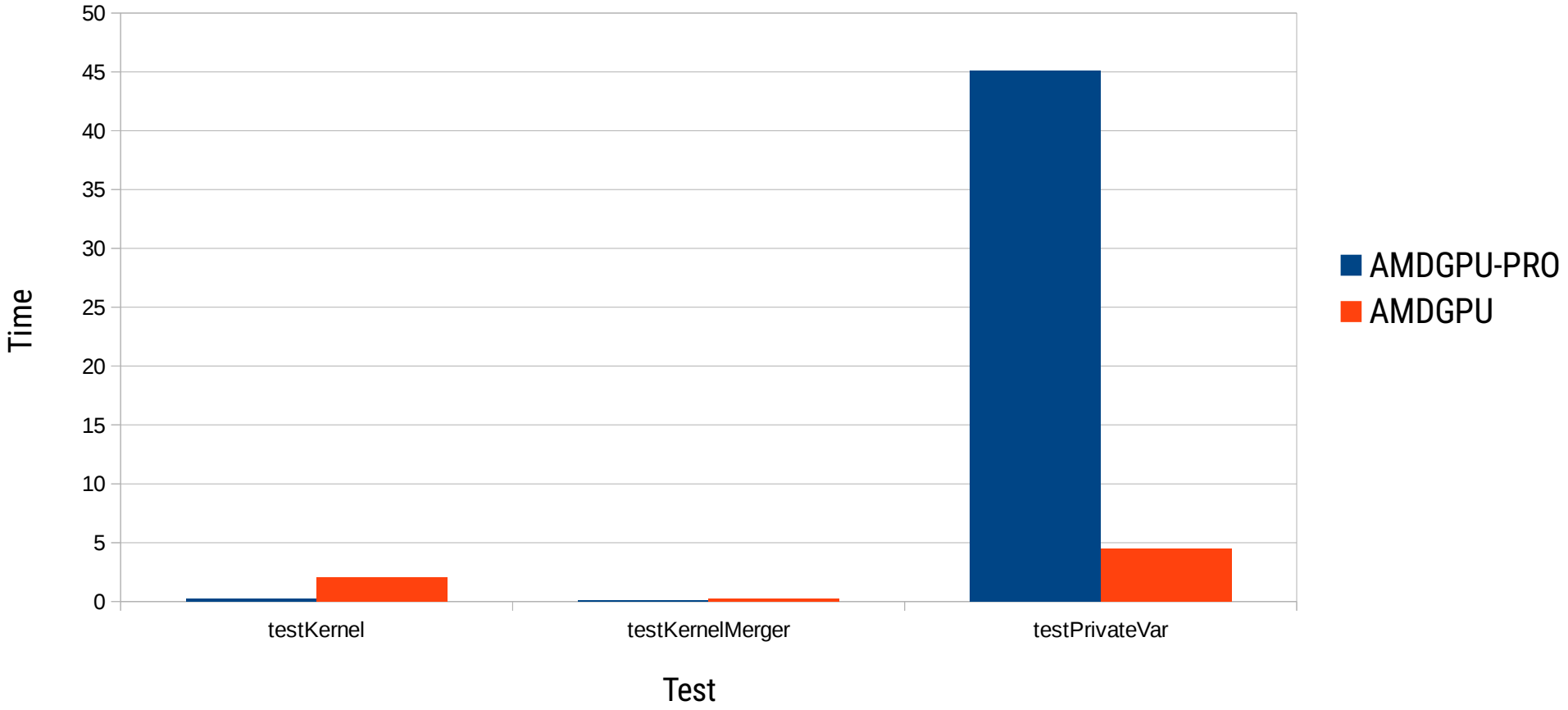
OpenMM test execution time



LAMMPS example execution time



ASL test execution time



Other OpenCL software

- Blender
  - Different users report performance issues and crashes
- BEAGLE, phylogenetics library
  - Made some progress
- clBLAS and clFFT
  - Implmented clEnqueueFillBuffer, requires more work
  - Required for Octopus (quantum chem), probably others

Other OpenCL software

- BOINC, CP2K, Theano
  - Had users tell me “I would try it if worked”
- clpeak, opencl-stream, SNU NPB
  - Benchmarks
- App or lib you care about?

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