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

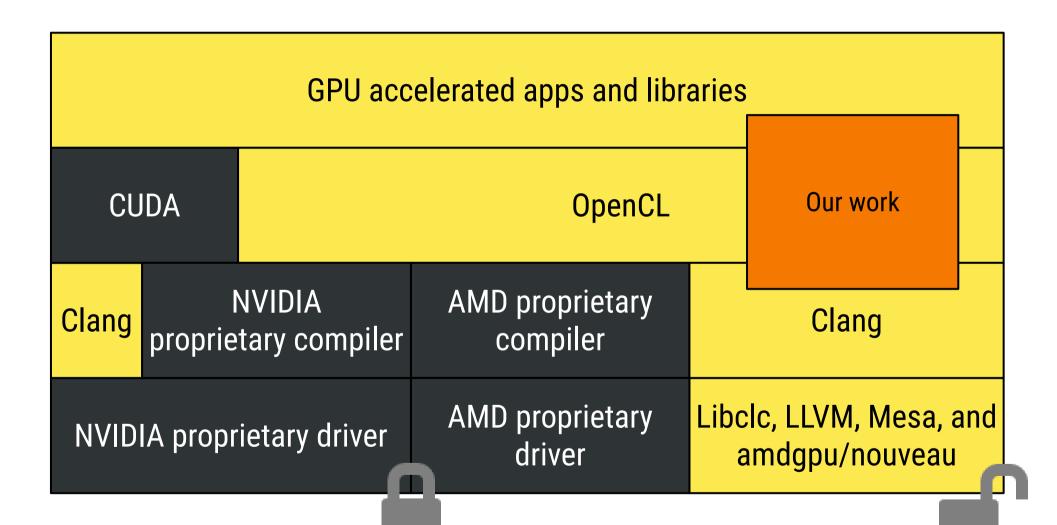
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Heidelberg Institute for Theoretical Studies





# Layers of GPU computing

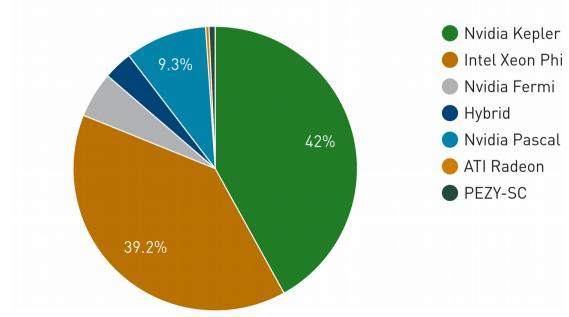


# State of the art: CUDA and OpenCL

#### CUDA

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

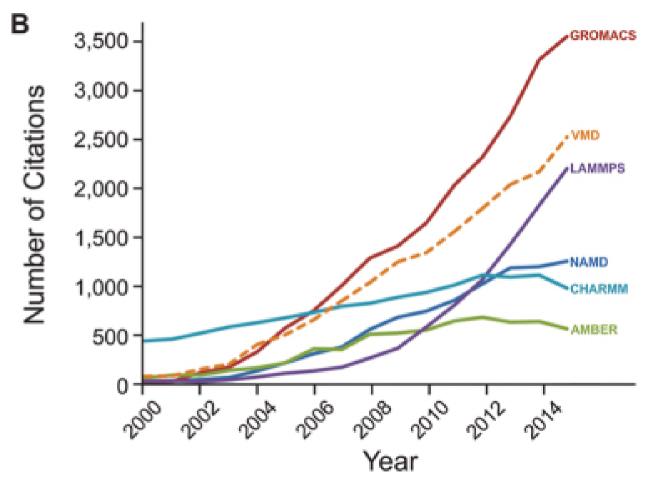
#### Accelerator/CP Family Performance Share



#### 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™

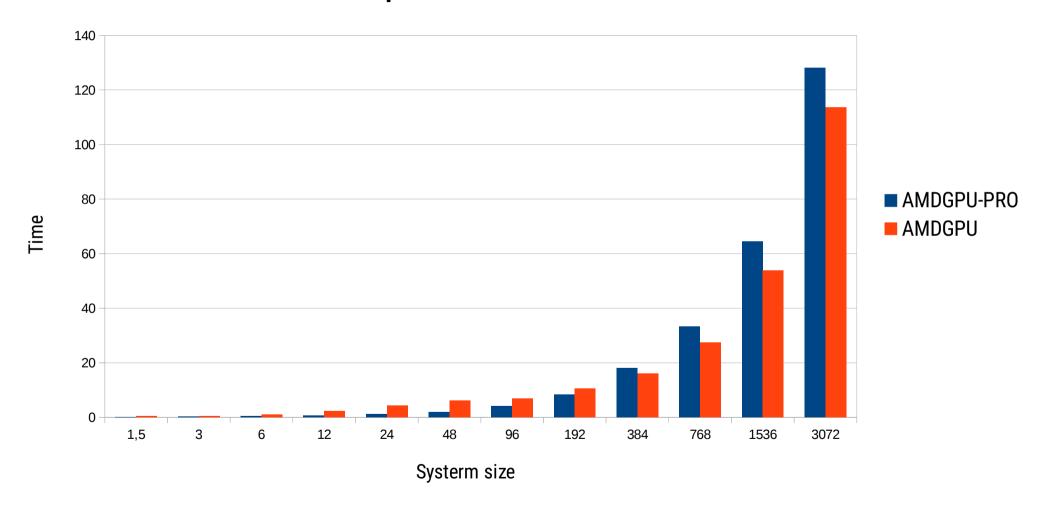
#### Mesa/LLVM

- AMD GPUs released 2009 or later
- Open source from the beginning<sup>™</sup>

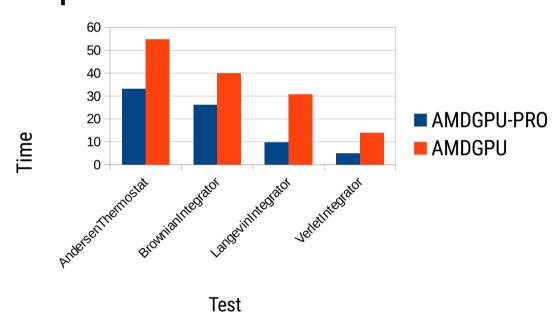
### Our work

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

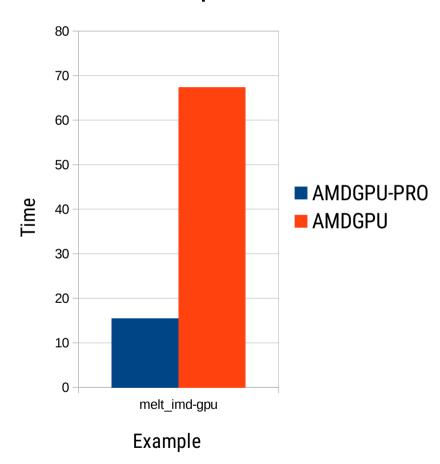
#### GROMACS OpenCL kernel execution time



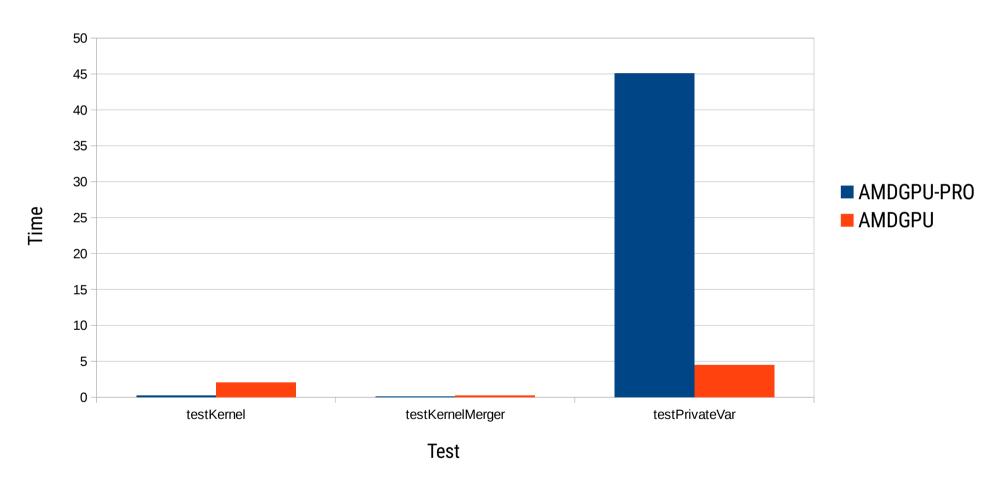
#### OpenMM test execution time



#### 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?

# Acknowledgments

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