Python based software on MIC

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What’s unique about my tuning work

- GPAW, wiki.fysik.dtu.dk/gpaw/
  - Python based open source software for electronic structure calculations in materials and nanoscience
  - High level algorithms in Python, kernels in C or in libraries

- Native / offload execution

- Intel compilers, Vtune, Python profile module
Performance

- Significant amount of time is spent in BLAS routines
  - Matrix multiplications with very skew matrices (i.e. $64^3 \times 512$)
- No benefits from automatic offload by MKL
- Porting Python to MIC for native execution
  - In native mode, serial bottlenecks kill the performance
- Special pyMIC module for offloading (collaboration with M. Klemm)
  - Allocation of arrays on device from Python and data transfers between host and device
  - Launching offload kernels from Python code
  - First results promising, specific parts of a calculation can be accelerated by a factor of 2-6
Insights

- Amdahl’s law restricts severely usability of native execution
- Minimizing data transfer between host and device is critical for offload performance
- Remaining challenges:
  - Efficient MIC versions for key C-kernels
  - MPI version of GPAW supporting multiple devices