

Python based software on MIC

Jussi Enkovaara
Senior Application Scientist
CSC – IT Center for Science
Espoo, Finland



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