Quantum ESPRESSO on GPU accelerated systems

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Outline

- Introduction and objectives
- Quantum ESPRESSO (QE) / PWscf
- GPU implementation in CUDA Fortran
- Benchmarking and Results
- Conclusions

Introduction

- First-principle computer simulations of materials are routinely used in academia and industry to understand their physical properties
- High performance computing (HPC) systems are required to study large systems and/or reduce the time to solution
- GPU-accelerated systems are now very popular in HPC:
    - GPUs are many-core processors with high flop rate and memory BW
    - GPUs are very energy efficient
    - Mature software ecosystem (compilers, math libraries, profiler/debugger)

Objectives

- Porting of QE PWscf to GPU using CUDA Fortran
    - Single source code for CPU and GPU
    - Extensive use of kernel loop directives (CUF kernels)
    - Validation and performance analysis on GPU systems with both x86 and Power host CPUs
    - All open source to show community best practices.

Quantum ESPRESSO/PWscf

Quantum ESPRESSO (QE)

- Integrated suite of open-source software for simulations of materials based on density-functional theory
- Popular package widely used within academia and industry
- PWscf: One of the main programs distributed with QE
    - Computes the Kohn-Sham (KS) orbitals and energies of material systems
    - Uses an iterative method that seeks self-consistent input and output charge densities

Plane-Wave Self-Consistent Field (PWscf)

- Each iteration requires:
    - Diagonalization of the Hamiltonian operator H_{KS}
        - done iteratively using a block Davidson method
        - performed for each KS orbital (***k*-point**) across *bands*
    - Computation of output charge density using diagonalization results
- Repeated until self-consistency is obtained within a desired tolerance

Parallelization Options

- PWscf has a number of parallelization options available. Options used in this study:
  - *k*-point parallelization using `-npool`:
    - Distributes *k*-points into N_K pools of processes.
    - Enables parallel execution of the iterative diagonalizations.
  - Linear algebra parallelization using `-ndiag`:
    - Distributes the dense diagonalization, needed by the block Davidson algorithm, among N_D processes.
    - Enables use of distributed eigensolver like ScaLAPACK

GPU Implementation in CUDA Fortran

CUDA Fortran

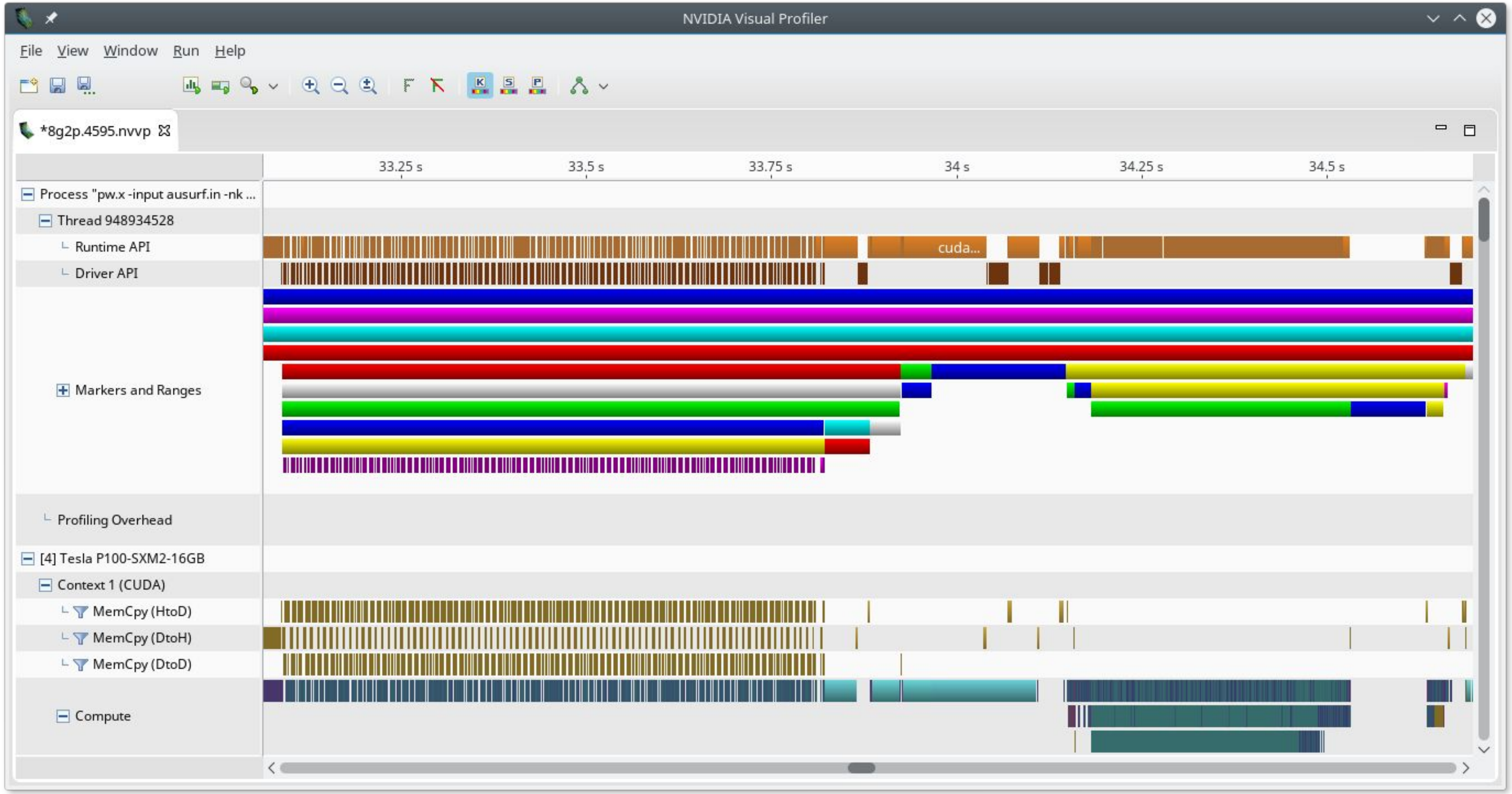
- Since baseline CPU code is written in Fortran, natural choice for GPU port is CUDA Fortran.
- Benefits:
    - More control than OpenACC:
        - Explicit GPU kernels written natively in Fortran are supported
        - Full control of host/device data movement
    - Directive-based programming available via CUF kernels
    - Easier to maintain than mixed CUDA C and Fortran approaches
- Requires PGI compiler (community edition available for free)

Profiling

- When porting programs, profiling (and profiling often) is very important:
    - Identify and focus efforts on performance-critical sections of the program
    - Understand interactions between CPU and GPU:
        - Am I getting expected H2D/D2H BW over PCIe or NVLink?
        - Can I hide this data movement behind GPU computation?
    - Understand library behavior:
        - How is my linked MPI library handling communication between GPUs?
        - Is the CPU being used in any library computations?

Profiling with NVPROF + NVVP + NVTX

- NVPROF:
  - Can be used to gather detailed kernel properties and timing information
- NVIDIA Visual Profiler (NVVP):
  - Graphical interface to visualize and analyze NVPROF generated profiles
  - Does not show CPU activity out of the box
- NVIDIA Tools EXtension (NVTX) markers:
  - Enables annotation with labeled ranges within program
  - Useful for categorizing parts of profile to put activity into context
  - Can be used to visualize normally hidden CPU activity (e.g. MPI communication)
- NVTX markers added to existing QE timing routines



Sample NVVP segment from AUSURF112 on NVIDIA DGX-1 System

GPU Porting of Key Computational Routines

- The iterative diagonalization and computation of charge density are dominated by three basic operation types:
  - Level-3 BLAS routines, predominantly `Z/DGEMM`
  - 3D Fast Fourier Transforms (FFT), typically distributed
  - dense-matrix diagonalization via LAPACK or ScaLAPACK
- BLAS routines easily ported using available routines in CUBLAS library
- 3D FFT and dense-matrix diagonalization more involved
- Remaining routines ported to GPU as necessary for performance or to remove redundant host/device data movement

3D Fast Fourier Transforms

- Required in iterative diagonalization and charge computation
- Component 1D FFT computations computed using CUFFT
- Generally distributed among the processes in each *k*-point pool:
  - requires transposition and data communication across processes using `MPI_Alltoall` or similar communication pattern
  - Many 3D FFT computations for each *k*-point, one for each band index

3D Fast Fourier Transforms

- Existing CPU implementation not amenable to a performant GPU port:
  - Individual FFTs for each band too small to saturate GPU resources
  - No attempt to overlap FFT computation with MPI communication:
    - problematic on GPU systems in cases where communication buffers must be staged through the host
- To address these issues, implemented a batched FFT strategy where multiple band FFTs computed together
  - More available concurrent work for better GPU utilization
  - Provides straightforward mechanism for pipelining data movement and computation
  - Requires more memory, but this was not an issue in tested cases

3D Fast Fourier Transforms

- As a further optimization, implemented all-to-all communication using non-blocking `MPI_Isend`/`MPI_Irecv`
  - Important on systems which are capable of multiple concurrent peer-to-peer (P2P) transfers between GPUs
- A number of MPI distributions we tried showed suboptimal utilization of available P2P bandwidth on systems with multiple P2P connections
  - For all-to-all, implemented explicit handling of P2P communication using CUDA interprocess communication (IPC), with non-peer transfers handled by linked MPI library

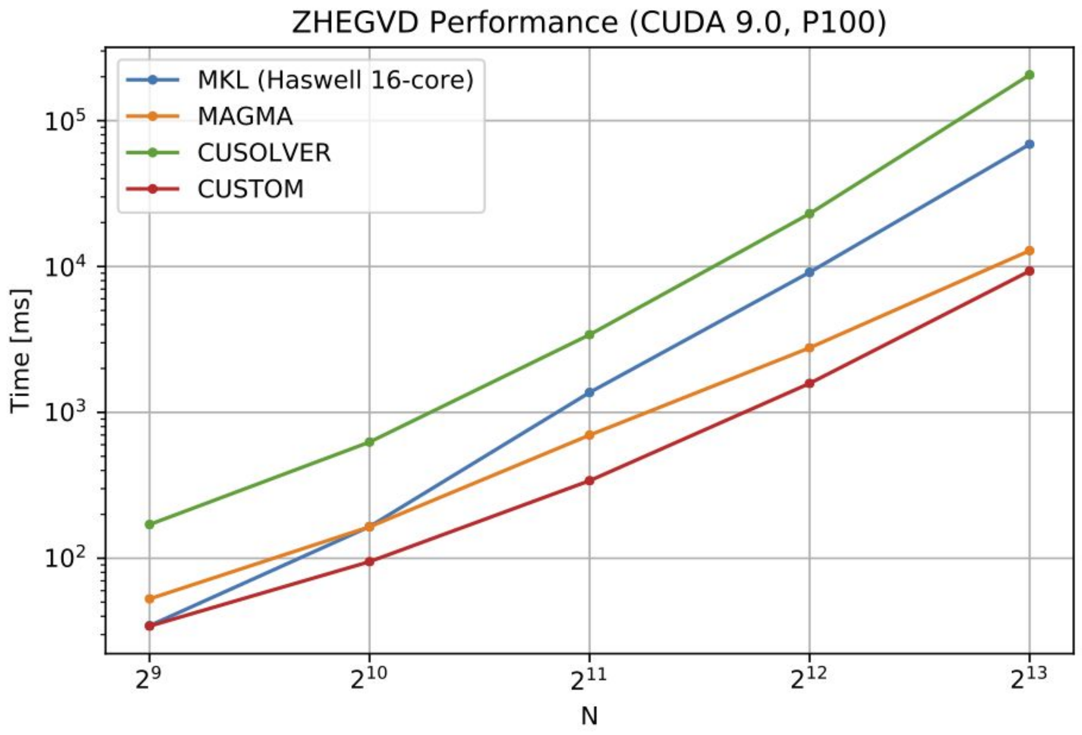
Diagonalization

- The dense-matrix diagonalization, used for the block Davidson method, is another computationally expensive routine.
- Consists of computing eigenvalues and eigenvectors of a modest size system (N x N with $N \sim O(10^3)$) using a dense eigensolver
- On CPU, this operation is typically distributed over N_D processes and computed using ScaLAPACK, or similar library

Diagonalization

- Current GPU port targets serial path (N_D = 1) using a custom developed GPU eigensolver
    - one GPU per k-point pool performs the dense-matrix diagonalization
- Custom solver used in lieu of several existing options for GPU, like MAGMA:
    - Written to reduce dependencies on CPU resources for computation, only reduced tridiagonal solve completed on CPU using LAPACK
    - Beneficial on “fat” nodes, with high GPU to CPU socket ratios, where bottlenecks due to limited CPU resources can arise

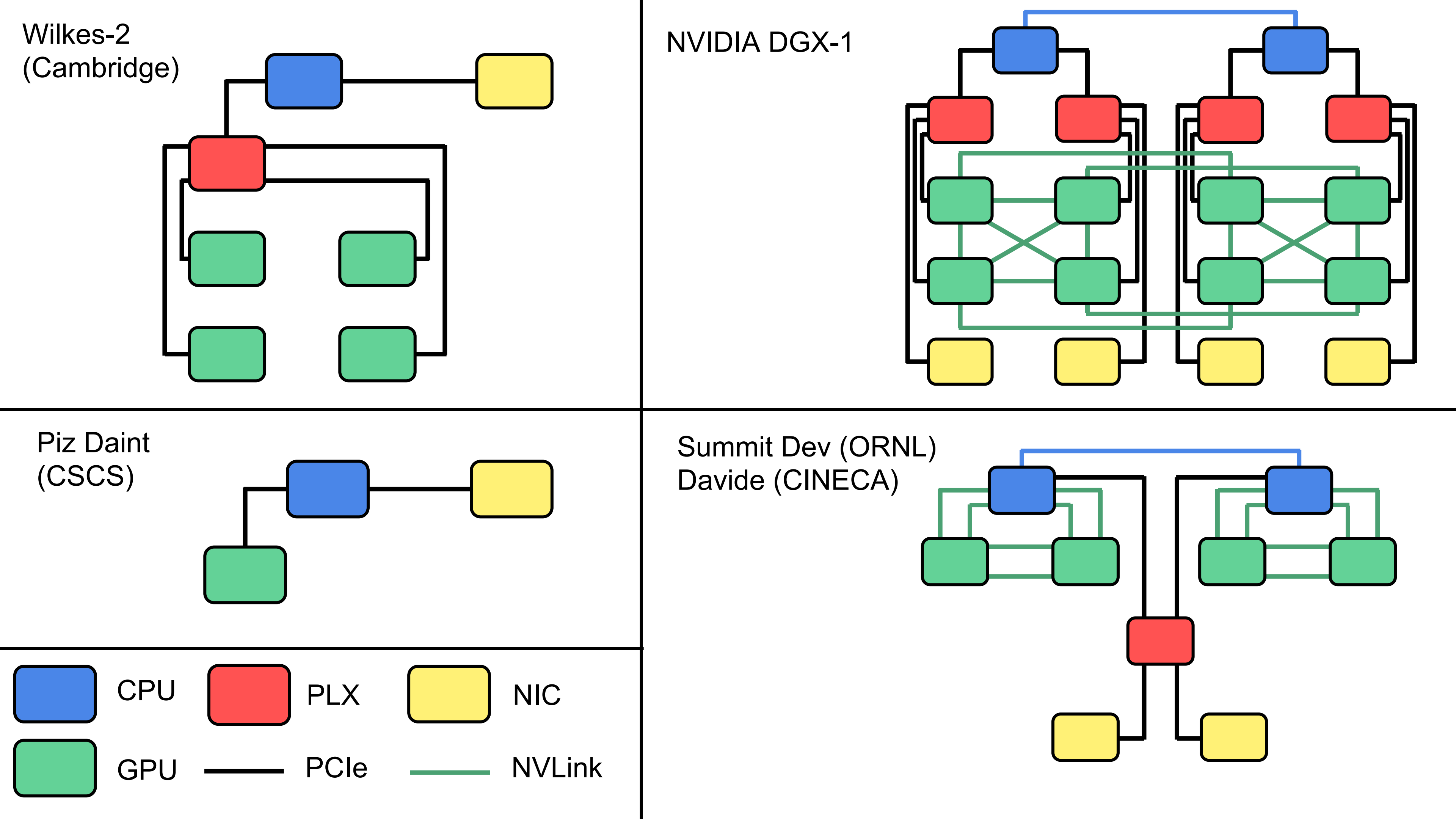
Diagonalization



Benchmarking and Results

Testing Details

- Performance results for three benchmark cases were obtained on several GPU systems and a reference CPU system.
- On reference CPU system:
  - Distributed ELPA solver used for diagonalization ($N_D > 1$)
  - MKL for other BLAS/LAPACK routines
  - OpenMP enabled, tried many configurations with best cases reported
- On GPU systems:
  - Custom serial eigensolver used for diagonalization ($N_D = 1$)
  - CUBLAS for BLAS routines on GPU, MKL/ESSL for any BLAS/LAPACK CPU routines
  - GDR features tested on systems with P2P connectivity (CUDA-aware MPI + custom IPC)
  - OpenMP enabled on Intel-based systems
  - OpenMP disabled on IBM system in favor of using multithreaded ESSL


Wilkes-2
(Cambridge)
NVIDIA DGX-1
Piz Daint
(CSCS)
Summit Dev (ORNL)
Davide (CINECA)
CPU
PLX
NIC
GPU
PCIe
NVLink

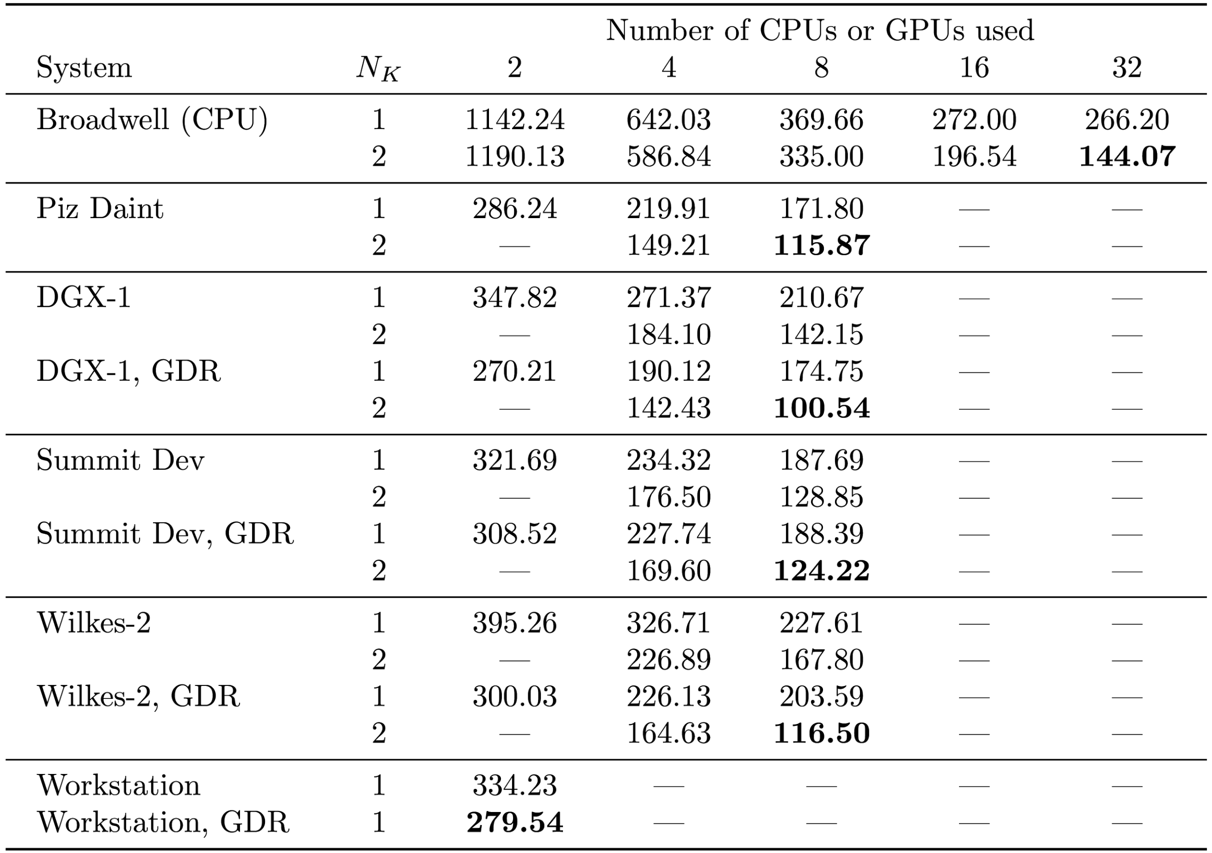
Benchmark Cases

- AUSURF112 (PWscf):
  - Gold surface with 112 atoms and 2 *k*-points
  - Smaller case suitable for workstations and small distributed systems
- Ta2O5 (PWscf):
  - Tantalum pentoxide with 96 atoms and 26 *k*-points.
  - Larger case suitable for scaling from small to large distributed systems
- Si63Ge (vc-relax)

	Benchmark case	
Parameter	AUSURF112	Ta2O5
Number of atomic species	1	2
Number of atoms	112	96
Number of electrons	$1,232$	544
Number of Kohn-Sham states	739	326
Number of k-points	2	26
Number of plane waves	$100,747$	$477,247$
Kinetic energy cutoff	25 Ry	130 Ry
Charge density cutoff	200 Ry	520 Ry
Dimension of dense FFT grid	$\{180, 90, 288\}$	$\{198, 168, 220\}$

AUSURF112: PWscf Time

- Factor of 2-3 speedup using GPU relative to CPU system
- Fixing number of resources per pool gives nearly linear scaling with increased resources
- Increasing number of resources per pool less efficient



		Number of CPUs or GPUs used				
System	N_K	2	4	8	16	32
Broadwell (CPU)	1	1142.24	642.03	369.66	272.00	266.20
	2	1190.13	586.84	335.00	196.54	**144.07**
Piz Daint	1	286.24	219.91	171.80	—	—
	2	—	149.21	**115.87**	—	—
DGX-1	1	347.82	271.37	210.67	—	—
	2	—	184.10	142.15	—	—
DGX-1, GDR	1	270.21	190.12	174.75	—	—
	2	—	142.43	**100.54**	—	—
Summit Dev	1	321.69	234.32	187.69	—	—
	2	—	176.50	128.85	—	—
Summit Dev, GDR	1	308.52	227.74	188.39	—	—
	2	—	169.60	**124.22**	—	—
Wilkes-2	1	395.26	326.71	227.61	—	—
	2	—	226.89	167.80	—	—
Wilkes-2, GDR	1	300.03	226.13	203.59	—	—
	2	—	164.63	**116.50**	—	—
Workstation	1	334.23	—	—	—	—
Workstation, GDR	1	**279.54**	—	—	—	—

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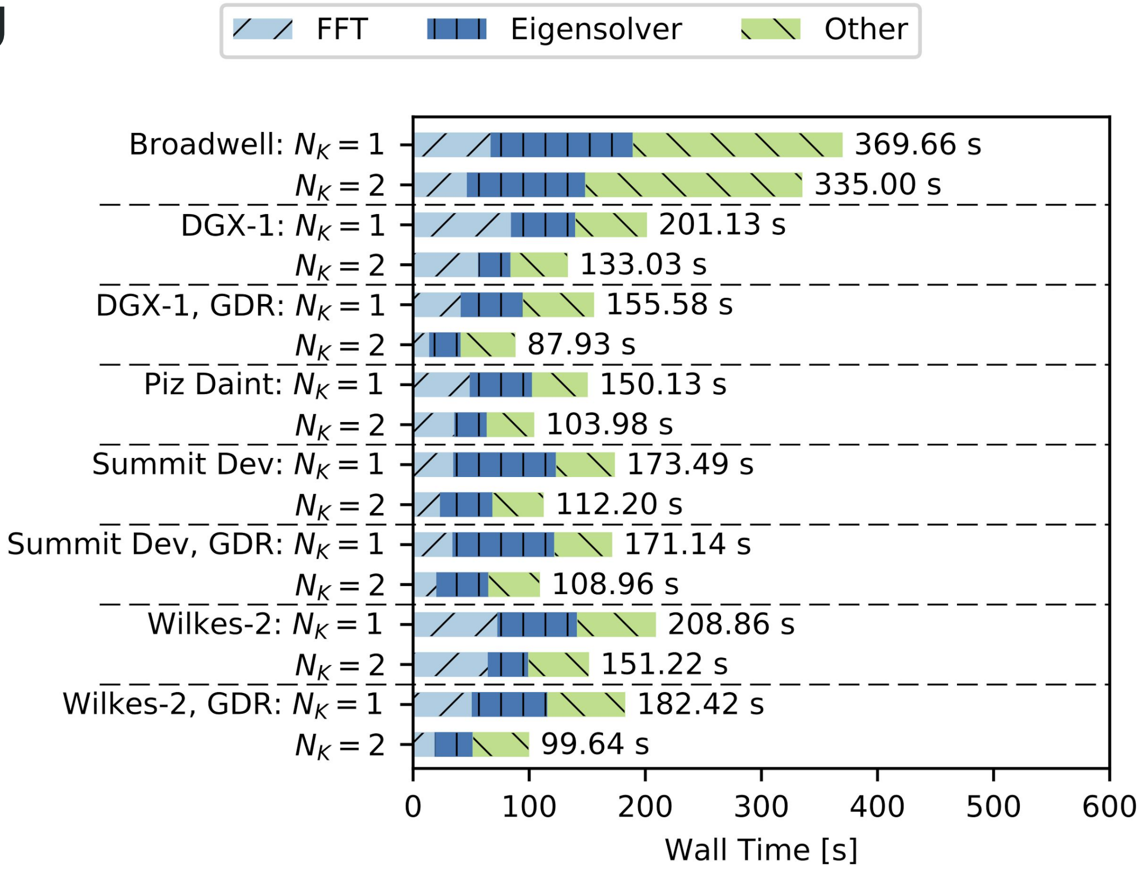
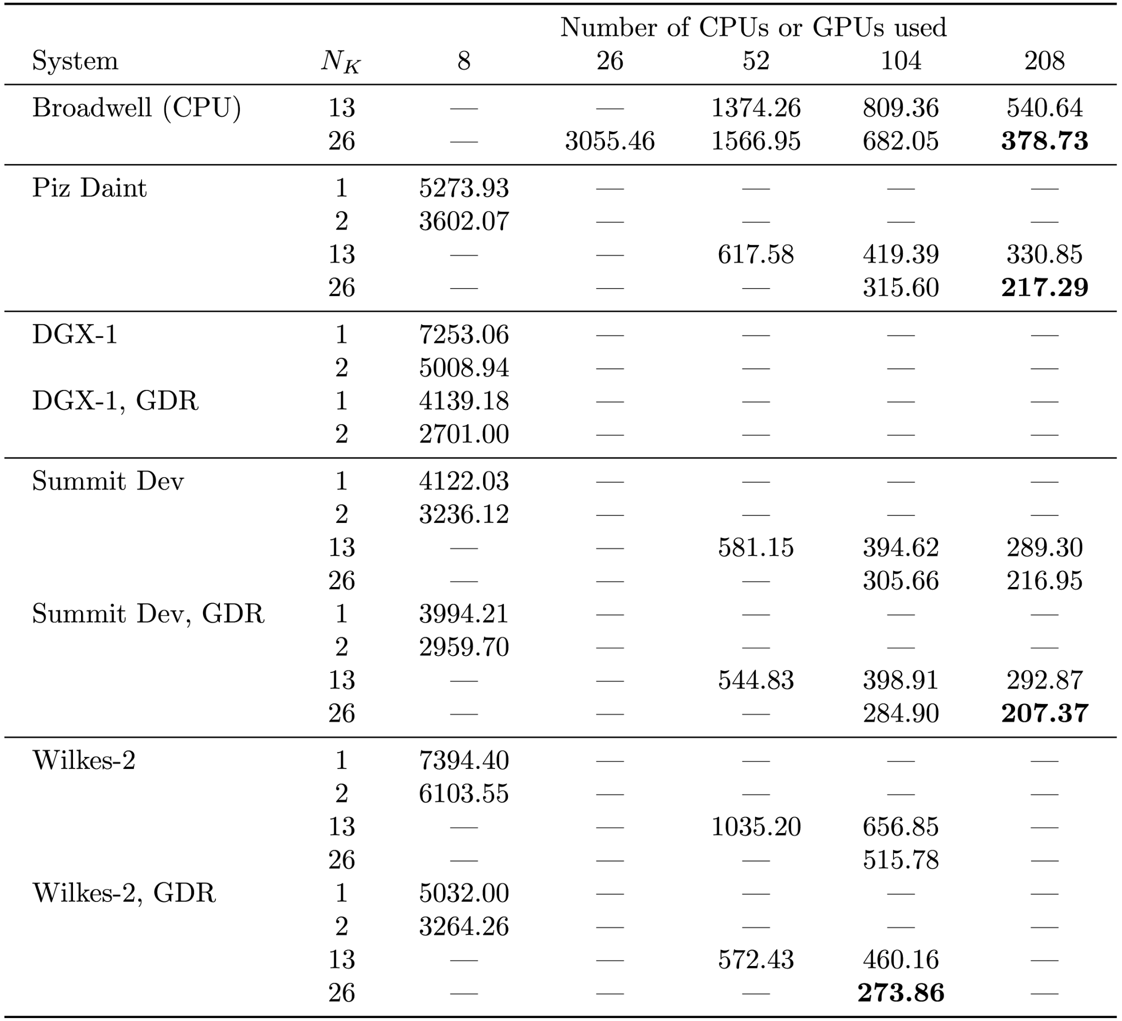
AUSURF112: 8 GPU/CPU

- GPU vs. CPU systems:
    - Faster performance on GPU systems
    - GPU eigensolver outperforming ELPA
- GPU systems:
    - FFT performance improvement with GDR
    - Eigensolver on Summit Dev slower than on Intel systems, more consistent across Intel systems



Ta2O5: PWscf Time

- Similar performance trends to AUSURF112 case
- Larger number of available *k*-points allows for scaling out further



System	N_K	Number of CPUs or GPUs used 8	26	52	104	208
Broadwell (CPU)	13	—	—	1374.26	809.36	540.64
	26	—	3055.46	1566.95	682.05	**378.73**
Piz Daint	1	5273.93	—	—	—	—
	2	3602.07	—	—	—	—
	13	—	—	617.58	419.39	330.85
	26	—	—	—	315.60	**217.29**
DGX-1	1	7253.06	—	—	—	—
	2	5008.94	—	—	—	—
DGX-1, GDR	1	4139.18	—	—	—	—
	2	2701.00	—	—	—	—
Summit Dev	1	4122.03	—	—	—	—
	2	3236.12	—	—	—	—
	13	—	—	581.15	394.62	289.30
	26	—	—	—	305.66	216.95
Summit Dev, GDR	1	3994.21	—	—	—	—
	2	2959.70	—	—	—	—
	13	—	—	544.83	398.91	292.87
	26	—	—	—	284.90	**207.37**
Wilkes-2	1	7394.40	—	—	—	—
	2	6103.55	—	—	—	—
	13	—	—	1035.20	656.85	—
	26	—	—	—	515.78	—
Wilkes-2, GDR	1	5032.00	—	—	—	—
	2	3264.26	—	—	—	—
	13	—	—	572.43	460.16	—
	26	—	—	—	**273.86**	—

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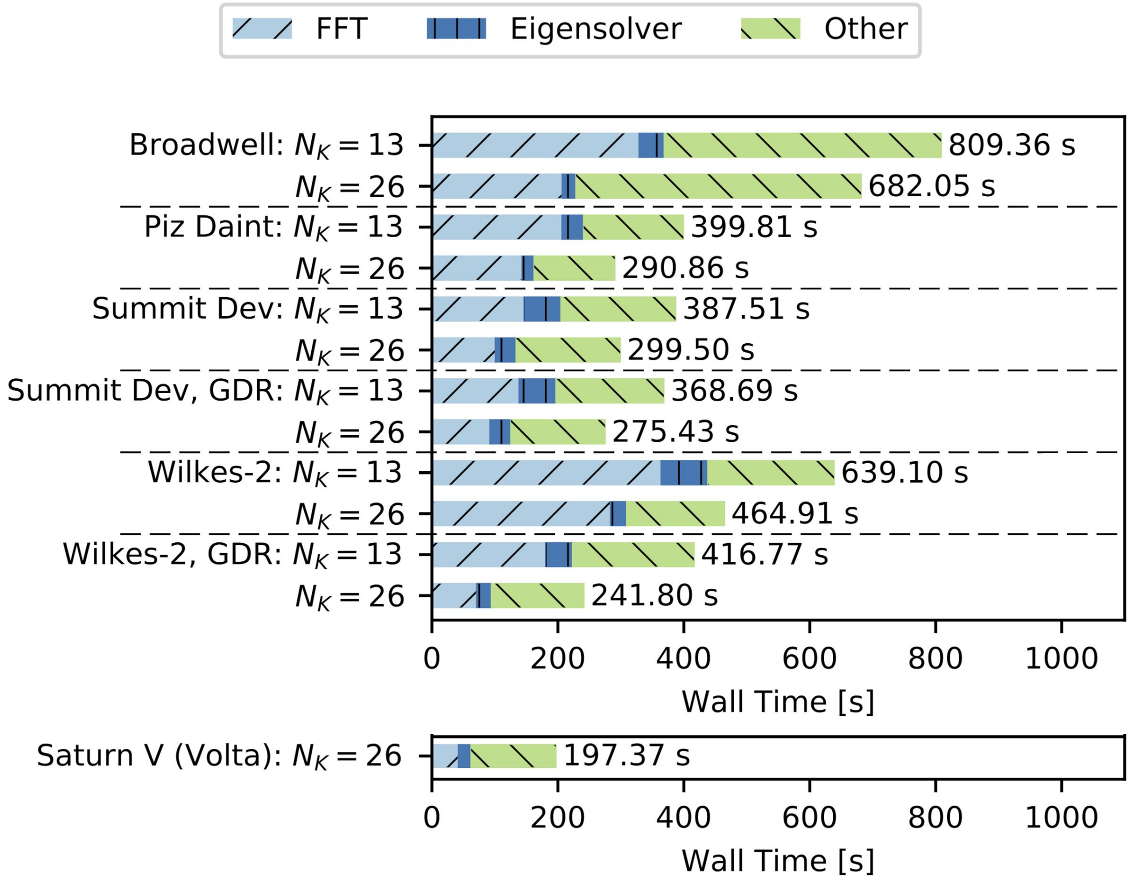
	26	—	—	—	**273.86**	—

Ta2O5: 104 GPU/CPU

- GPU vs. CPU systems:
  - ELPA faster in this case, but GPU eigensolver remains competitive

- GPU systems:
  - On fat systems, GDR required for high FFT performance
  - Summit Dev has high FFT performance without GDR due to host-device NVLink



Si63Ge (vc-relax)

	QE-GPU CSCS		QE CSCS	QE Cineca	
	1 P100	10 P100	20 BW (360c)	1 KNL (60c)	10 KNL (640c)
npool	1	10	10	5	10
init_run	15.92s	7.50s	4.45s	21.61s	10.33s
electrons	668.06s	108.78s	235.58s	1542.72s	292.86s
update_pot	1.37s	1.04s	10.42s	31.95s	7.94s
forces	12.06s	3.03s	13.20s	60.91s	11.93s
stress	74.28s	15.82s	75.69s	260.82s	38.55s
cdiaghg	71.38s	6.89s	15.51s	147.97s	76.15s
PWSCF	**774.49s**	**138.70s**	**342.26s**	**1934.28s**	**400.29s**

Fermi energy	6.5908 ev	6.5908 ev	6.5908 ev	6.5908 ev	6.5908 ev
Total energy	-813.93522903 Ry	-813.93522903 Ry	-813.93522904 Ry	-813.93522904 Ry	-813.93522903 Ry
Total force	0.002992	0.002992	0.002992	0.002992	0.002992
Total stress	0.00000062	0.00000062	0.00000062	0.00000062	0.00000062
Pressure	0.09	0.09	0.09	0.09	0.09

BW/KNL results from *https://github.com/electronic-structure/benchmarks*

Si63Ge (vc-relax)

	QE-GPU CSCS		QE-GPU	Sirius GPU CSCS	
	1 P100	10 P100	1 V100	1 P100	1 P100
npool	1	10	1	1	10
init_run	15.92s	7.50s	11.06s		
electrons	668.06s	108.78s	501.46s	1014.01s	156.48s
update_pot	1.37s	1.04s	0.59s		
forces	12.06s	3.03s	8.58s	28.86s	3.85s
stress	74.28s	15.82s	52.58s	94.95s	12.99s
cdiaghg	71.38s	6.89s	84.10s	147.97s	76.15s
PWSCF	**774.49s**	**138.70s**	**576.02s**	**1168.07s**	**190.25s**

Fermi energy	6.5908 ev	6.5908 ev	6.5908 ev	6.5916 ev	6.5916 ev
Total energy	-813.93522903 Ry	-813.93522903 Ry	-813.93522903 Ry	-813.94388964 Ry	-813.94389190 Ry
Total force	0.002992	0.002992	0.002992	0.003004	0.003004
Total stress	0.00000062	0.00000062	0.00000062	0.00000078	0.00000078
Pressure	0.09	0.09	0.09	0.11	0.11

BW/KNL/SIRIUS results from *https://github.com/electronic-structure/benchmarks*

Conclusions

Conclusions

- New GPU implementation can reduce time to solution by a factor of 2 - 3 relative to the reference CPU system.
- Code runs on both x86 and Power systems with GPU
- Custom serial GPU eigensolver provides competitive performance relative to ScaLAPACK and ELPA with limited sensitivity to host resources. Available on Github at: *https://github.com/NVIDIA/Eigensolver_gpu*
- Full utilization of P2P resources essential for high performance, especially on systems with large GPU to CPU socket ratios
- CUDA-accelerated version of QE is open-source and available on Github at: *https://github.com/fspiga/qe-gpu*