JÜLICH
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HPC generation of the Hamiltonian and Overlap matrices in DFT methods based on linearized and augmented plane waves

JLESC, Kobe, December 1st 2016 | Edoardo di Napoli

Motivation

Code modernization

- Legacy codes in Materials Science have grown with focus on functionality
- Frequent problems:
  - Codes lacks modularity, encapsulation, code reuse, ...
  - Codes are often a direct translation of mathematical formulas
- Problems get exacerbated with recent shift to heterogeneous architectures
- “Modernize or perish”
  - Yes, it is costly
  - Yes, it is necessary but benefits are substantial

Goal

Performance portability

In general

- Re-engineering the software by re-thinking the algorithms;
- Modular design, clear layering and interfaces;
- Bottom layers: standardized and highly optimized libraries.

In this talk:

- the FLEUR code as use case
- Modernize a portion of the code that takes about 40% of the computation
- Required an important initial effort
- We now give evidence of performance portability to heterogeneous CPU + GPU architectures

Outline

The FLAPW method & FLEUR code

An exercise in performance portability

Experimental results

Conclusions

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Density Functional Theory (DFT)

1. $\Phi(x_1; s_1, x_2; s_2, \ldots, x_n; s_n) \Longrightarrow \Lambda_{i,a}\psi_a(x_i; s_i)$
2. **density of states** $n(\mathbf{r}) = \sum_a f_a \left|\psi_a(\mathbf{r})\right|^2$
3. In the Schrödinger equation the exact Coulomb interaction is substituted with an effective potential $V_0(\mathbf{r}) = V_{\mathrm{I}}(\mathbf{r}) + V_{\mathrm{H}}(\mathbf{r}) + V_{\mathrm{xc}}(\mathbf{r})$

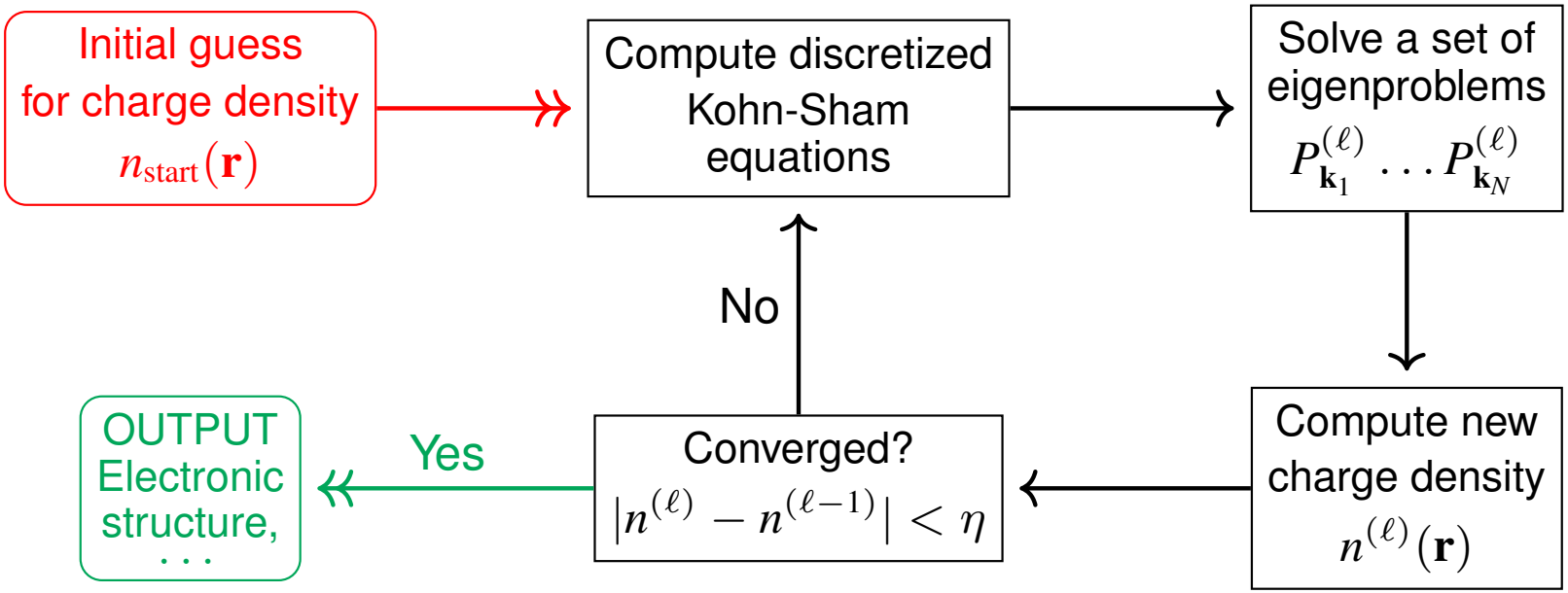
Hohenberg-Kohn theorem

- $\exists$ one-to-one correspondence $n(\mathbf{r}) \leftrightarrow V_0(\mathbf{r}) \quad \Longrightarrow \quad V_0(\mathbf{r}) = V_0(\mathbf{r})[n]$
- $\exists!$ a functional $E[n]$: $\quad E_0 = \min_n E[n]$

The high-dimensional Schrödinger equation translates into a set of coupled non-linear low-dimensional self-consistent Kohn-Sham (KS) equation

$$\forall\, a \quad \text{solve} \quad \hat{H}_{\mathrm{KS}}\psi_a(\mathbf{r}) = \left(-\frac{\hbar^2}{2m}\nabla^2 + V_0(\mathbf{r})\right)\psi_a(\mathbf{r}) = \epsilon_a\psi_a(\mathbf{r})$$

DFT self-consistent field cycle



Zoo of methods

LDA
GGA
LDA + U
Hybrid functionals
GW-approximation

Plane waves
Localized basis set
Real space grids
Green functions

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_0(\mathbf{r})\right)\psi_a(\mathbf{r}) = \epsilon_a\psi_a(\mathbf{r})$$

Finite differences
Non-relaticistic eqs.
Scalar-relativistic approx,
Spin-orbit coupling
Dirac equation

All-electron
Pseudo-potential
Shape approximations
Full-potential
Spin polarized p calculations

Introduction to FLAPW

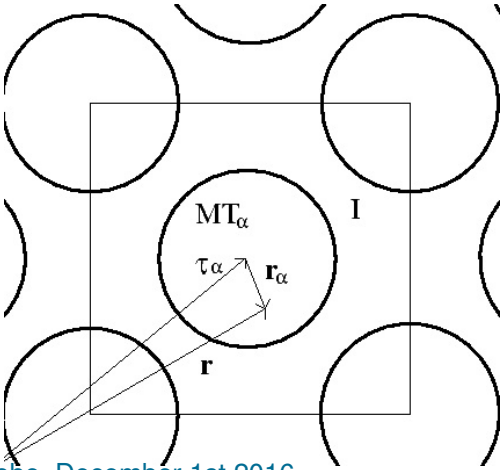
LAPW basis set

$$\psi_a(\mathbf{r}) = \sum_G^{N_G} c_{G,i}\varphi_G(\mathbf{r}) \qquad i = (\mathbf{k}, \nu)$$

$\mathbf{k}$ Bloch vector

ν band index

$$\varphi_G(\mathbf{r}) = \begin{cases} e^{i(\mathbf{k}+\mathbf{G}_t)\mathbf{r}} & \text{INT} \\ \sum_{\ell,m} \left[A^{a,G}_{(l,m)} u_{l,a}(r) + B^{a,G}_{(l,m)} \dot{u}_{l,a}(r)\right] Y_{l,m}(\hat{\mathbf{r}}_a) & a^{\text{th}}\ \text{MT} \end{cases}$$



boundary conditions

Continuity of wavefunction and its derivative at MT boundary

$\Downarrow$

$A^{a,G}_{(l,m)}$ and $B^{a,G}_{(l,m)}$

Hamiltonian and Overlap matrices

Operatorial form

$$(H)_{G',G} = \sum_a \iint \varphi^*_{G'}(\mathbf{r}) \hat{H}_{\mathrm{KS}} \varphi_G(\mathbf{r}) \mathrm{d}\mathbf{r}, \quad (S)_{G',G} = \sum_a \iint \varphi^*_{G'}(\mathbf{r}) \varphi_G(\mathbf{r}) \mathrm{d}\mathbf{r}.$$

Entrywise form

$$(S)_{G',G} = \sum_a \sum_{L=(l,m)} \left(A_L^{a,G'}\right)^* A_L^{a,G} + \left(B_L^{a,G'}\right)^* B_L^{a,G} \left\|\dot{u}_{l,a}\right\|^2$$

$$(H)_{G',G} = \sum_a \sum_{L',L} \left(\left(A_{L'}^{a,G'}\right)^* T^{[AA]}_{L',L;a} A_L^{a,G}\right) + \left(\left(A_{L'}^{a,G'}\right)^* T^{[AB]}_{L',L;a} B_L^{a,G}\right)$$
$$+ \left(\left(B_{L'}^{a,G'}\right)^* T^{[BA]}_{L',L;a} A_L^{a,G}\right) + \left(\left(B_{L'}^{a,G'}\right)^* T^{[BB]}_{L',L;a} B_L^{a,G}\right).$$

Hamiltonian and Overlap matrices

Matrix form

$$H = \sum_{a=1}^{N_A} \underbrace{A_a^H T_a^{[AA]} A_a}_{H_{AA}} + \underbrace{A_a^H T_a^{[AB]} B_a + B_a^H T_a^{[BA]} A_a + B_a^H T_a^{[BB]} B_a}_{H_{AB+BA+BB}}$$

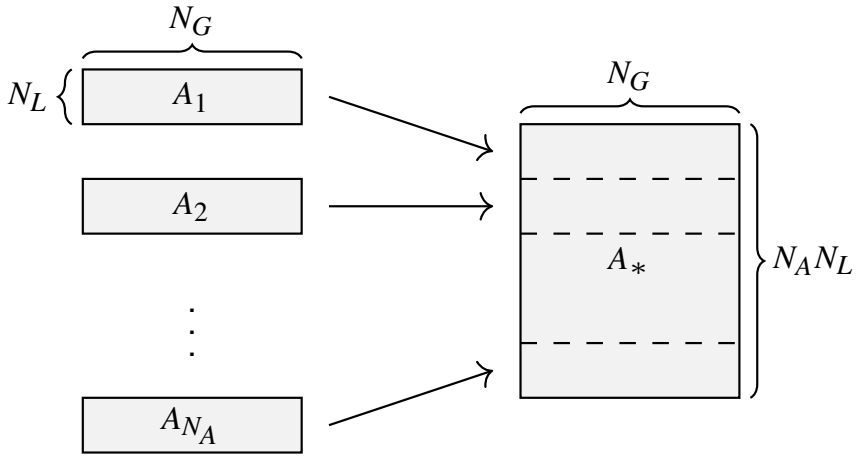
$$S = \underbrace{\sum_{a=1}^{N_A} A_a^H A_a}_{S_{AA}} + \underbrace{\sum_{a=1}^{N_A} B_a^H \dot{U}_a^H \dot{U}_a B_a}_{S_{BB}}$$

Constructing S_{AA}

An example of memory layout re-structuring

$$S_{AA} = \sum_{a=1}^{N_A} A_a^H A_a.$$

1: **for** $a := 1 \rightarrow N_A$ **do**
2: $\quad S_{AA} = A_a^H A_a$ ▷ (`zherk`: $4N_L N_G^2$ Flops)
3: **end for**



1: $S_{AA} = A_\star^H A_\star$ ▷ (`zherk`: $4N_A N_L N_G^2$ Flops)

Constructing $H_{AB+BA+BB}$

An example of algorithm re-structuring

$$H_{AB+BA+BB} = \sum_{a=1}^{N_A} B_a^H (T_a^{[BA]} A_a) + (A_a^H T_a^{[AB]}) B_a +$$
$$\frac{1}{2} B_a^H (T_a^{[BB]} B_a) + \frac{1}{2} (B_a^H T_a^{[BB]}) B_a$$
$$= \sum_{a=1}^{N_A} B_a^H (T_a^{[BA]} A_a + \frac{1}{2} T_a^{[BB]} B_a) +$$
$$(A_a^H T_a^{[AB]} + \frac{1}{2} B_a^H T_a^{[BB]}) B_a$$

1: **for** $a := 1 \rightarrow N_A$ **do**
2: $\quad Z_a = T_a^{[BA]} A_a$ ▷ (`zgemm`: $8 N_L^2 N_G$ Flops)
3: $\quad Z_a = Z_a + \frac{1}{2} T_a^{[BB]} B_a$ ▷ (`zhemm`: $8 N_L^2 N_G$ Flops)
4: $\quad$ Stack Z_a to $Z_\star$ and B_a to $B_\star$
5: **end for**
6: $H = Z_\star^H B_\star + B_\star^H Z_\star$ ▷ (`zher2k`: $8 N_A N_L N_G^2$ Flops)

Stripped HSDLA algorithm for H and S

1: Create A, B
2: // $H_{AB+BA+BB}$
3: **for** $a := 1 \rightarrow N_A$ **do**
4: $\quad Z_a = T_a^{[BA]} A_a$ ▷ (`zgemm`: $8N_L^2 N_G$ Flops)
5: $\quad Z_a = Z_a + \frac{1}{2} T_a^{[BB]} B_a$ ▷ (`zhemm`: $8N_L^2 N_G$ Flops)
6: **end for**
7: $H = Z^H B + B^H Z$ ▷ (`zher2k`: $8N_A N_L N_G^2$ Flops)
8: // S
9: $S = A^H A$ ▷ (`zherk`: $4N_A N_L N_G^2$ Flops)
10: $B = UB$ ▷ (`scaling`: $2N_A N_L N_G$ Flops)
11: $S = S + B^H B$ ▷ (`zherk`: $4N_A N_L N_G^2$ Flops)
12: // H_{AA}
13: **for** $a := 1 \rightarrow N_A$ **do**
14: $\quad$ **try:**
15: $\quad\quad C_a = Cholesky(T_a^{[AA]})$ ▷ (`zpotrf`: $\frac{4}{3} N_L^3$ Flops)
16: $\quad$ **success:**
17: $\quad\quad Y_a = C_a^H A_a$ ▷ (`ztrmm`: $4N_L^2 N_G$ Flops)
18: $\quad$ **failure:**
19: $\quad\quad X_a = T_a^{[AA]} A_a$ ▷ (`zhemm`: $8N_L^2 N_G$ Flops)
20: **end for**
21: $H = H + A^H_{\neg \mathrm{HPD}} X_{\neg \mathrm{HPD}}$ ▷ (`zgemm`: $8N_{A_{\neg \mathrm{HPD}}} N_L N_G^2$ Flops)
22: $H = H + Y^H_{\mathrm{HPD}} Y_{\mathrm{HPD}}$ ▷ (`zherk`: $4N_{A_{\mathrm{HPD}}} N_L N_G^2$ Flops)

Previous multi-core results

NaCl ($\mathbf{K}_{\max} = 4.0$)	IvyBridge			Haswell		
	HSDLA	FLEUR	×	HSDLA	FLEUR	×
1 core	31.53	48.31	**1.53**	19.00	47.41	**2.50**
2 cores	16.10	24.58	**1.53**	9.98	24.95	**2.50**
1 CPU	3.90	6.21	**1.59**	2.25	5.00	**2.22**
2 CPUs	2.61	5.20	**1.99**	1.93	4.03	**2.09**
TiO_2 ($\mathbf{K}_{\max} = 3.6$)	IvyBridge			Haswell		
	HSDLA	FLEUR	×	HSDLA	FLEUR	×
1 core	175.53	256.15	**1.46**	106.56	259.91	**2.44**
2 cores	86.68	127.90	**1.48**	53.48	131.21	**2.45**
1 CPU	19.63	29.35	**1.50**	10.63	25.95	**2.44**
2 CPUs	12.25	21.50	**1.76**	7.55	16.76	**2.22**

Table: Scalability of HSDLA and FLEUR: execution times in minutes on Haswell (12 cores / CPU) and IvyBridge (10 cores / CPU); speedups of HSDLA over FLEUR in **bold**.

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An exercise in performance portability

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Porting to heterogeneous architectures

- Re-wrote the generation of H and S in terms of standardized libraries
- Reached a speedup of around $2\times$
- Can one exploit this useful excercize in code modernization beyond the speed obtained?

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Kernels-based algorithms go a long way

- BLAS is the first numerical library ported to every new architecture
- On paper: quick and easy port to other architectures
- The natural questions are:
  - Can one port to CPU+GPU with minimal modifications?
  - How far can one get in terms of performance improvements?

Porting to heterogeneous architectures

Back-of-the-envelope analysis

- 5 lines of the algorithm constitute 97% of flops
- Correspond to BLAS-3 operations (`gemm, herk, her2k`)
- High arithmetic intensity and should fit GPUs well

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- First step: offload these routine calls
- All 5 are BLAS kernels. Can we use some library?
  - cuBLAS
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  - MAGMA
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Porting to heterogeneous architectures

Additional code?

3 x wrappers around the BLAS calls:

```
void gpu_zgemm_( char *transa, char *transb, int *m,  int *n, int *k,
                 std::complex<double> *alpha,  std::complex<double> *A,  int *lda,
                 std::complex<double> *B,  int *ldb,
                 std::complex<double> *beta, std::complex<double> *C,  int *ldc )
{
    cublasOperation_t cu_transa = transa[0] == 'N' ? CUBLAS_OP_N :
                                  transa[0] == 'T' ? CUBLAS_OP_T : CUBLAS_OP_C;
    cublasOperation_t cu_transb = transb[0] == 'N' ? CUBLAS_OP_N :
                                  transb[0] == 'T' ? CUBLAS_OP_T : CUBLAS_OP_C;
    cublasXtZgemm( handle, cu_transa, cu_transb, *m, *n, *k,
                   (cuDoubleComplex *)alpha, (cuDoubleComplex *)A, *lda,
                                             (cuDoubleComplex *)B, *ldb,
                   (cuDoubleComplex *)beta,  (cuDoubleComplex *)C, *ldc );
}
```

Porting to heterogeneous architectures

Additional code?

- 3x wrappers (zgemm, zherk, zher2k)
- Init and cleanup of cuda runtime and devices
  - Get #devices, initialize devices, create handlers, ...
  - Destroy handlers, free devices, ...
- Allocate data in page-locked memory
  - Avoid “hidden” copies
  - Fast data transfer

Porting to heterogeneous architectures

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Only around 100 lines of additional code

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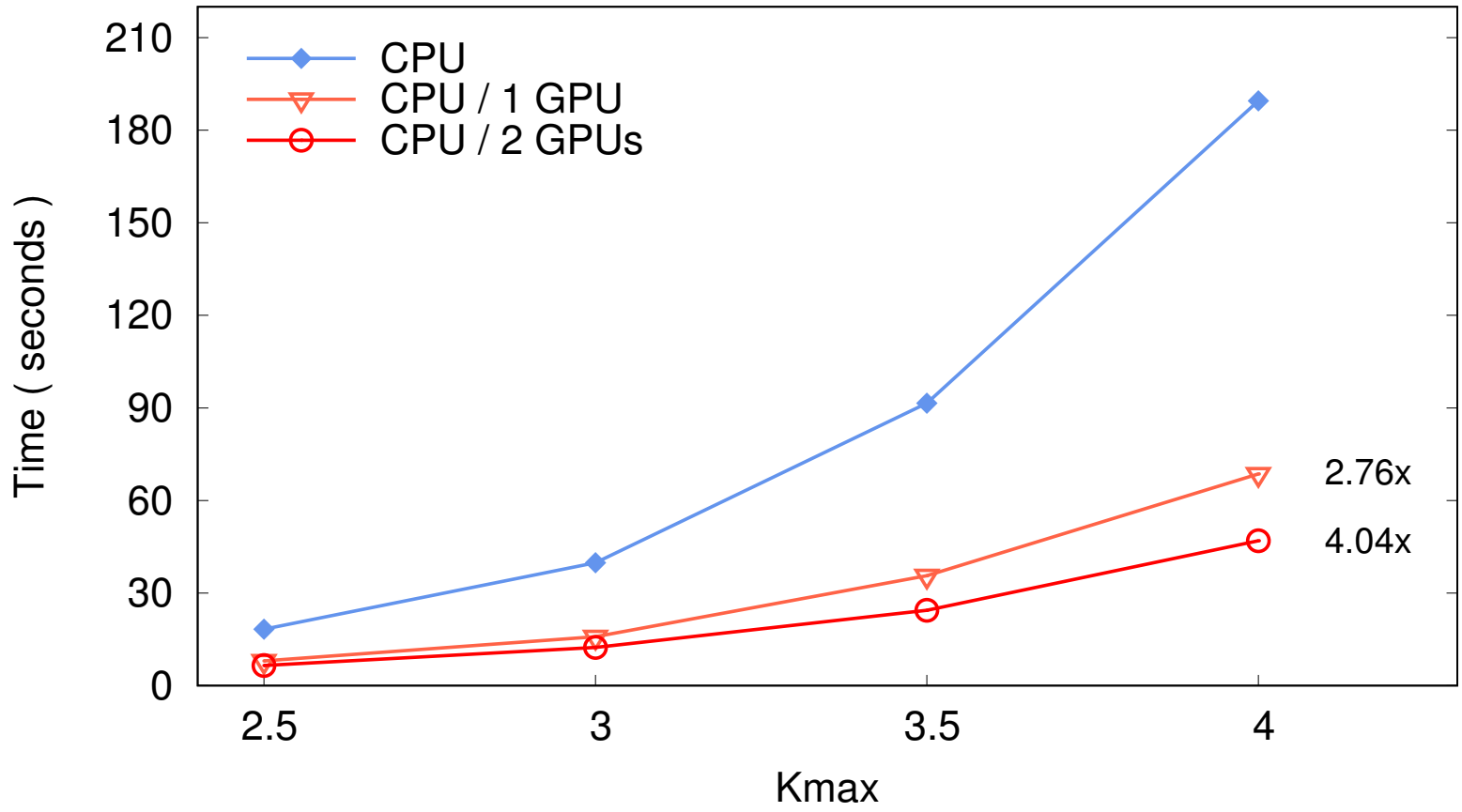
Experimental results

Sandy Bridge:

- CPU: E5-2650, 2 x 8core, 2.0GHz, 64GBs RAM
- 2 Nvidia Tesla K20X
- Peak performance: 256 GFs/s + 2 x 1.3 TFs/s

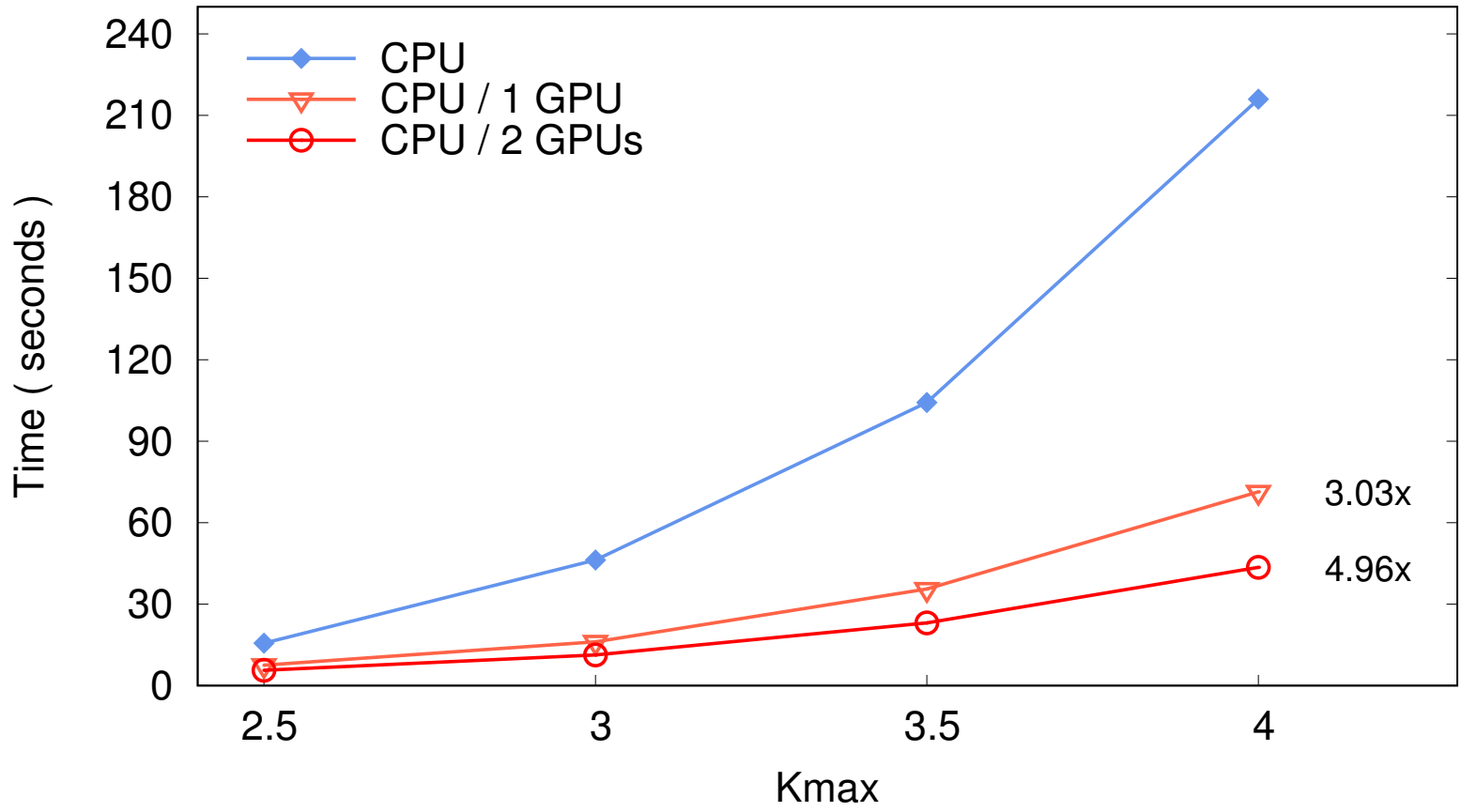
Experimental results

Test case 1: NaCl ($N_A = 512$, $N_L = 49$, $N_G = [2256 - 9273]$)



Experimental results

Test case 2: AuAg ($N_A = 108$, $N_L = 121$, $N_G = [3275 - 13379]$)



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- **Modernizing** algorithm structure of legacy code is critical
- Layered design built on top of standardized libraries
- Increase in performance
- (Almost) free lunch $\Rightarrow$ **performance portability**
- Case of FLEUR: up to 12 $\times$ speedup

Conclusions and Future Work

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- Case of FLEUR: up to 12 $\times$ speedup

Future Work:

- Hybrid for `zgemm`, `zherk`, `zher2k`
- Experiments on Jureca (4 GPU devices)
- **Apply the same methodology** to other Materials Science codes

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Thank you for your attention!

Details on the original HSDLA:

- “High-performance generation of the Hamiltonian and Overlap matrices in FLAPW methods.” *Edoardo Di Napoli, Elmar Peise, Markus Hrywniak and Paolo Bientinesi*. Accepted for publication in Comp. Phys. Comm. [arXiv:1602.06589]
- “Hybrid CPU-GPU generation of the Hamiltonian and Overlap matrices in FLAPW methods.” *Diego Fabregat-Traver, Davor Davidović, Markus Höhnerbach, Edoardo Di Napoli*.
  Accepted for publication in LNCS. [arXiv:1611.00606]