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Investigating the Performance Portability Capabilities of OpenMP 4.0, Kokkos and RAJA

Using TeaLeaf and other mini-apps to assess the performance portability of modern parallel programming models

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Agenda

- Which mini-apps?
- How do you program with each model?
- Which models perform best?
- Conclusions

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Mini-apps

TeaLeaf (2d)

Implicit, sparse, matrix-free solvers for heat conduction equation on structured grid, memory bandwidth bound

Solvers: Conjugate Gradient (CG), Chebyshev, Preconditioned Polynomial CG (PPCG)

CloverLeaf (2d)

Lagrangian-Eulerian hydrodynamics – explicit solver on structured grid, memory bandwidth bound

Bristol University Docking Engine (BUDE)

Molecular docking benchmark that uses an Evolutionary Monte Carlo technique, compute bound

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The Porting Process

- New ports with emerging parallel programming models:
  - **TeaLeaf**: *Kokkos, RAJA, OpenMP 4.0, OpenACC*
  - **CloverLeaf**: *OpenACC, OpenMP 4.0*
  - **BUDE**: *OpenACC, OpenMP 4.0*

- Developed or utilised existing ports to gauge performance bounds:
  - OpenCL, CUDA, OpenMP 3.0

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CUDA Code Sample

```
// CUDA kernel for CG solver
__global__ void cg_calc_p(/*...*/)
{
    // Get global id of thread
    int gid = threadIdx.x + blockIdx.x*blockDim.x;
    int col = gid % x;
    int row = gid / x;

    // Exclude halo region from computation
    if(col >= pad && col < x-pad && row >= pad && row < y-pad)
    {
        p[index] = r[index] + beta*p[index];
    }
}

// Execute with n blocks of 128 threads
cg_calc_p<<< n, 128 >>>(/*...*/);
```

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OpenMP 4.0 Code Sample

```
// Setup device data environment
#pragma omp target data \
    map(to: r[:r_len]) map(tofrom: p[:p_len])
{
    // Offload calculation using resident data
    #pragma omp target teams distribute
    for(int jj = pad; jj < y-pad; ++jj)
    {
        for(int kk = pad; kk < x-pad; ++kk)
        {
            int index = jj * x + kk;
            p[index] = beta * p[index] + r[index];
        }
    }
} // Only p is read back from device
```

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OpenMP 4.0 Alternatives

```
// CCE GPU targeting
#pragma omp target teams distribute
for(/*...*/) {}

// Intel KNC targeting
#pragma omp target
#pragma omp parallel for
for(/*...*/) {}

// Clang GPU targeting
#pragma omp target teams distribute
#pragma omp parallel for
for(/*...*/) {}
```

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RAJA Code Sample

```
// Global execution policy for IndexSets
typedef RAJA::IndexSet::ExecPolicy<
    RAJA::seq_segit, RAJA::omp_parallel_for_exec> policy;

// Custom box segment taking box coords
RAJA::BoxSegment box(/*...*/)
RAJA::IndexSet inner_domain_list;
inner_domain_list.push_back(box);

// Halo region excluded by virtue of the BoxSegment
RAJA::forall<policy>(inner_domain_list, [=] RAJA_DEVICE (int index)
{
    p[index] = beta*p[index] + r[index];
});
```

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Kokkos Code Sample

```
// Define the target device type
#define DEVICE Kokkos::OpenMP

// Globally initialise the execution space and views
Kokkos::Initialize();
Kokkos::View<double*, DEVICE> p("p", x*y);

Kokkos::parallel_for(x*y, KOKKOS_LAMBDA (int index)
{
    int kk = index % x;
    int jj = index / x;

    // Exclude halo region from computation
    if(kk >= pad && kk < x - pad && jj >= pad && jj < y - pad)
    {
        p(index) = beta*p(index) + r(index);
    }
});
```

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The Performance Experiment

- Performance tested on **CPU**, **GPU**, and **KNC**
- Single node only (multi-node scaling proven)
- All ports were optimised as much as possible, whilst aiming for performance portability
- Solved *4096x4096* problem, the point of mesh convergence, for *single iteration*

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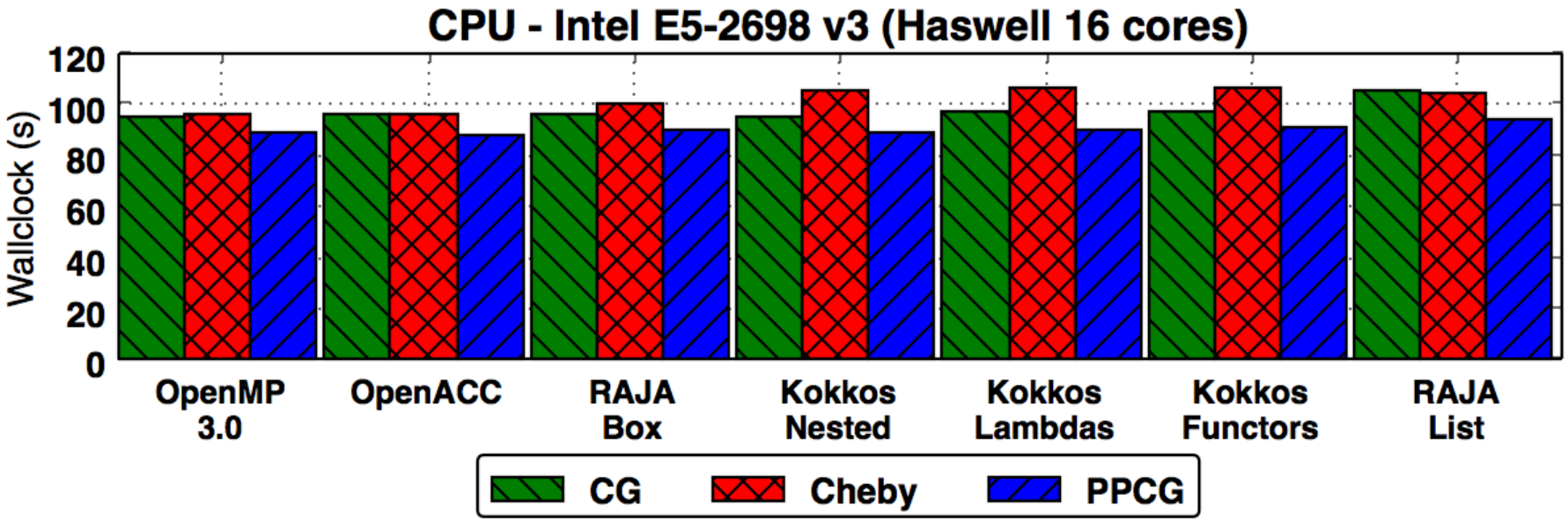
TeaLeaf - CPU



Intel Compilers 16.0.1 (OpenMP, Kokkos, RAJA), and PGI Compilers 15.10 (OpenACC)

At most 12% runtime penalty for modern Intel CPU, nearly identical relative performance seen with Ivy Bridge

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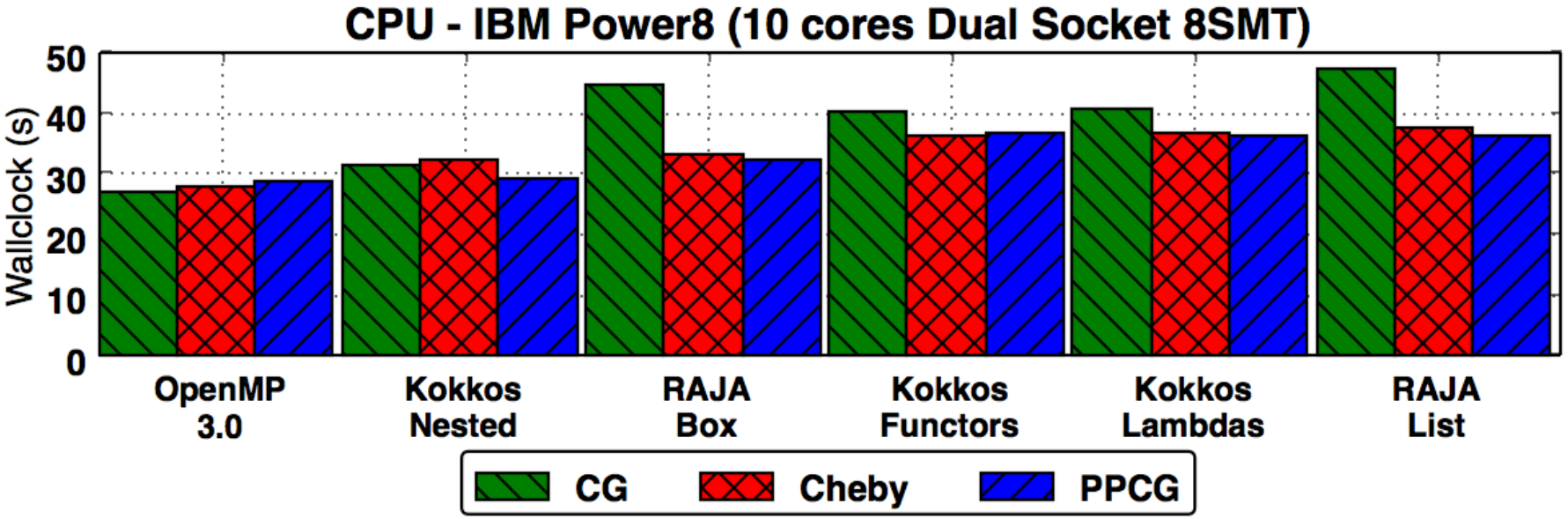
TeaLeaf – Power8



GCC 4.9.1 (OpenMP, Kokkos, RAJA)

Results generally good, and particularly for optimised Kokkos Nested and RAJA Box versions

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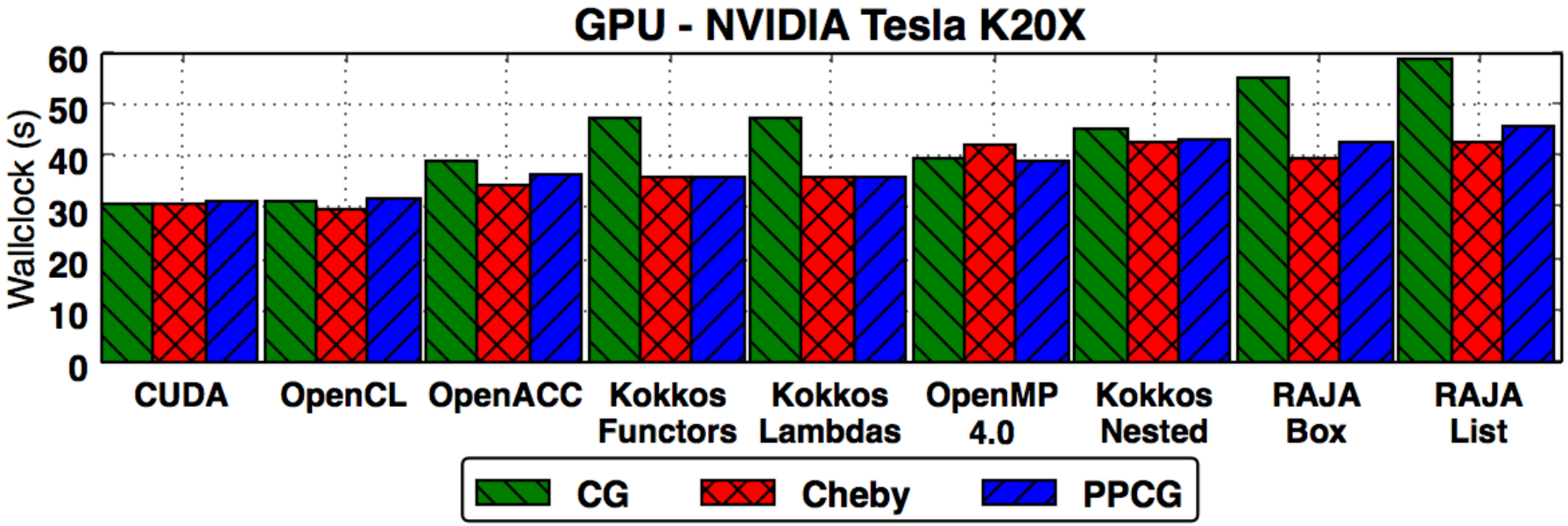
TeaLeaf – GPU



CUDA Toolkit 7.5 (All), PGI 15.10 (OpenACC), CCE 8.4.4 (OpenMP 4.0)

Performance bug with CG again present in some cases

Shows that all portable models have a small runtime penalty

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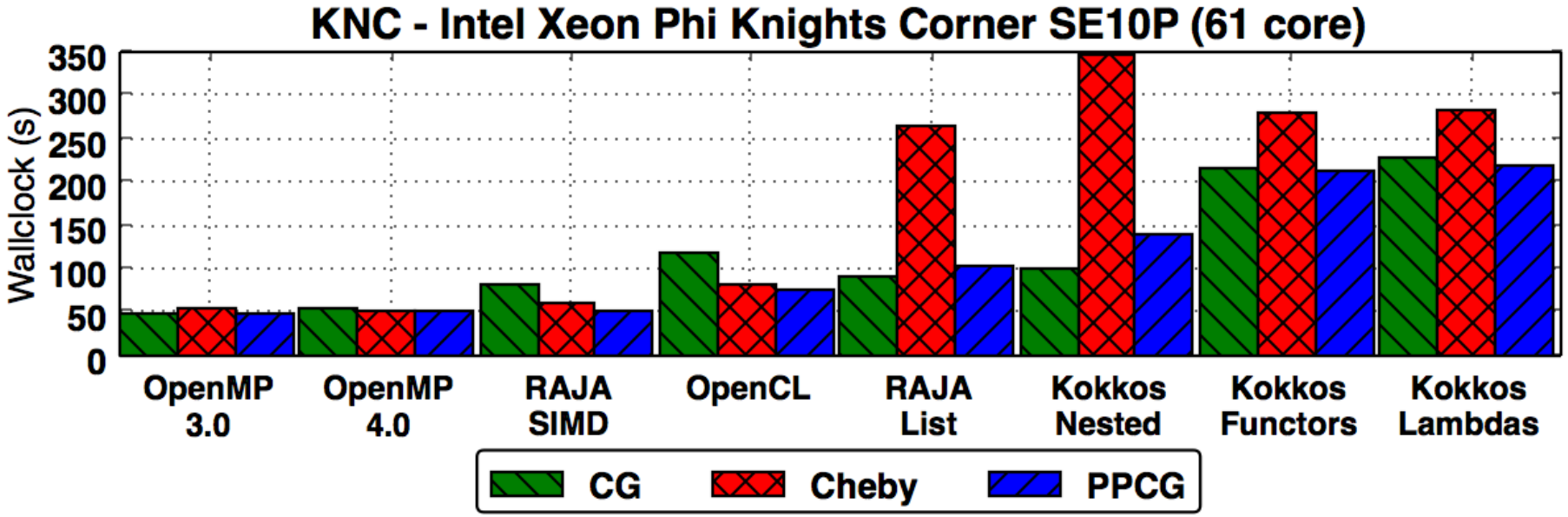
TeaLeaf – KNC



Intel Compilers 16.0.1 (OpenMP, RAJA, Kokkos), Intel OpenCL (OpenCL)

Achieving good performance is more challenging on KNC

Vectorisation was a very important factor

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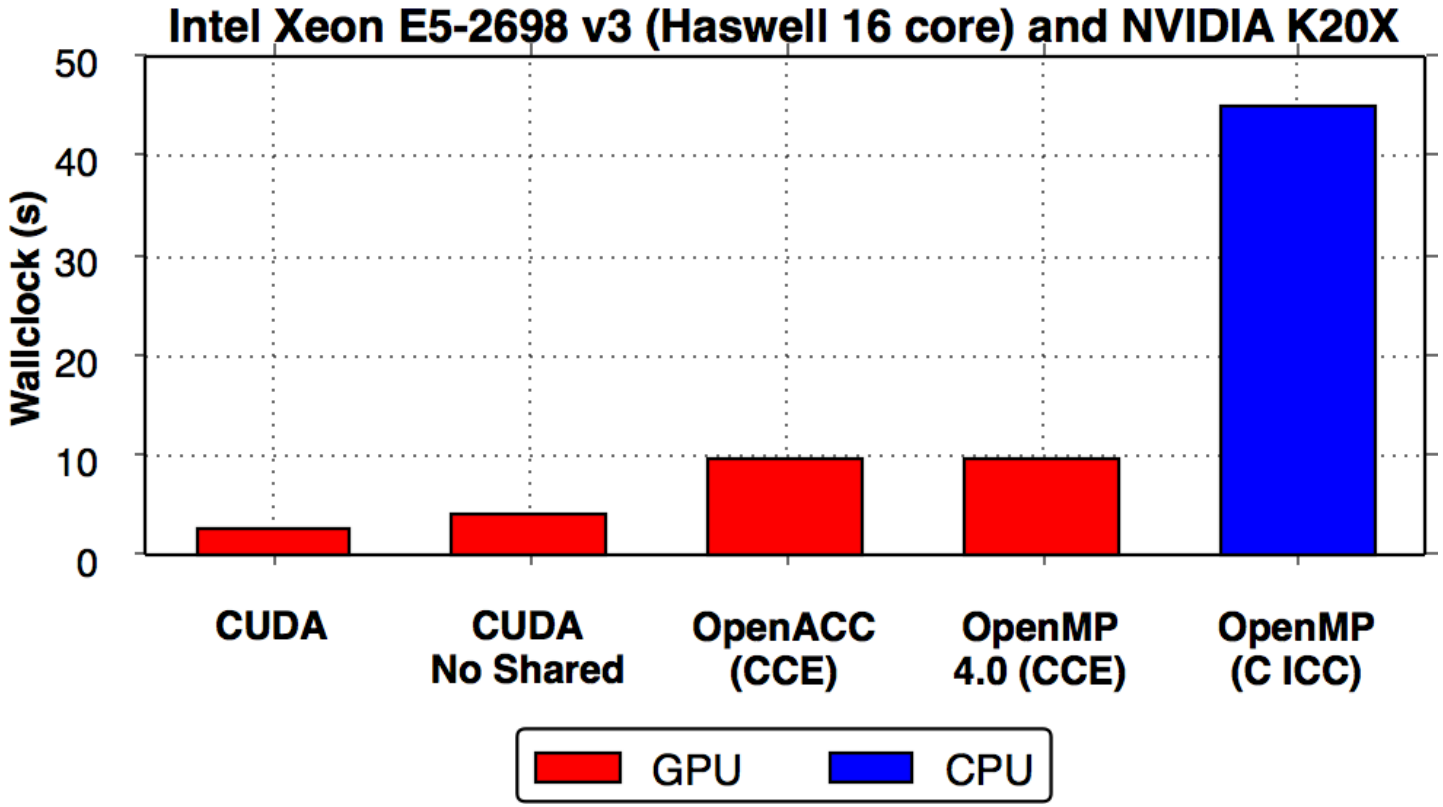
BUDE – CPU & GPU



Required at least 2.2x runtime, shared optimisation increased this even further

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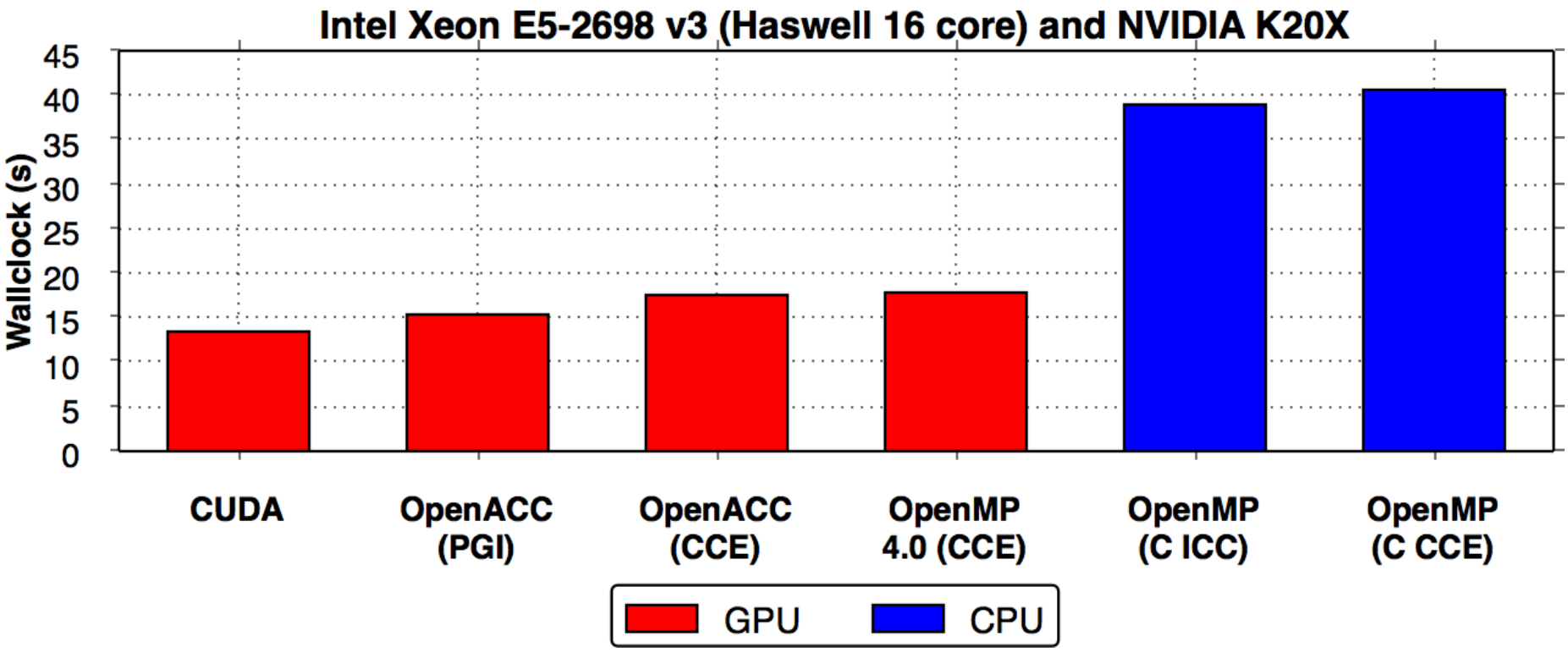
CloverLeaf – CPU & GPU



At most 1.3x performance penalty, re-emphasises good performance of directive-based models for such problems

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Conclusions

- There are already lots of maturing models
- You can balance performance and complexity
- The performance portable models can achieve performance that is close to low-level APIs
- **Your** best choice might depend on:
  - Productivity and potential for tuning
  - The dominant language of your applications

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Any Questions?

Mini-apps including TeaLeaf, CloverLeaf, SNAP (for GPUs), and BUDE
https://github.com/UK-MAC/
https://github.com/UoB-HPC/

Assessing the Performance Portability of Modern Parallel Programming Models using TeaLeaf
Martineau, M., McIntosh-Smith, S. & Gaudin, W.
Submitted to Concurrency and Computation: Practice and Experience (April 2016)

Optimising Sparse Iterative Solvers for Many-Core Computer Architectures
Boulton, M., McIntosh-Smith S., Gaudin, W., & Garrett, P. Presented at UKMAC'14, Cambridge, December 2014

Evaluating OpenMP 4.0's Effectiveness as a Heterogeneous Parallel Programming Model
Martineau, M., McIntosh-Smith, S. & Gaudin, W.
Presenting at HIPS Workshop (IPDPS), Chicago, May 2016

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Extra Slides

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SNAP

- High dimensionality and sweep presents an interesting difficulty for many models
- We were not able to accelerate with CCE on GPU because of use of indirection arrays
- OpenACC using PGI does successfully achieve within 50% runtime of hand-optimised CUDA implementation