ICHEC
Irish Centre for High-End Computing

Hybrid CUDA/OpenMP Porting of the Non-Bonded Force-Field for Two-Body Systems

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Introduction

- DL_POLY
  - General purpose serial and parallel molecular dynamics simulation package.
  - Daresbury Labs UK
- OpenMP/CUDA Port
  - Accelerated components:
    - Two-body force field, link cells, metal forces/potentials, electrostatics, shake velocity verlet, etc.
  - Reproduces the non-CUDA results
  - Supports self-tuning host/device overlap.
  - Tesla/Fermi optimised.

Two-Body Force Field Algorithm (1)

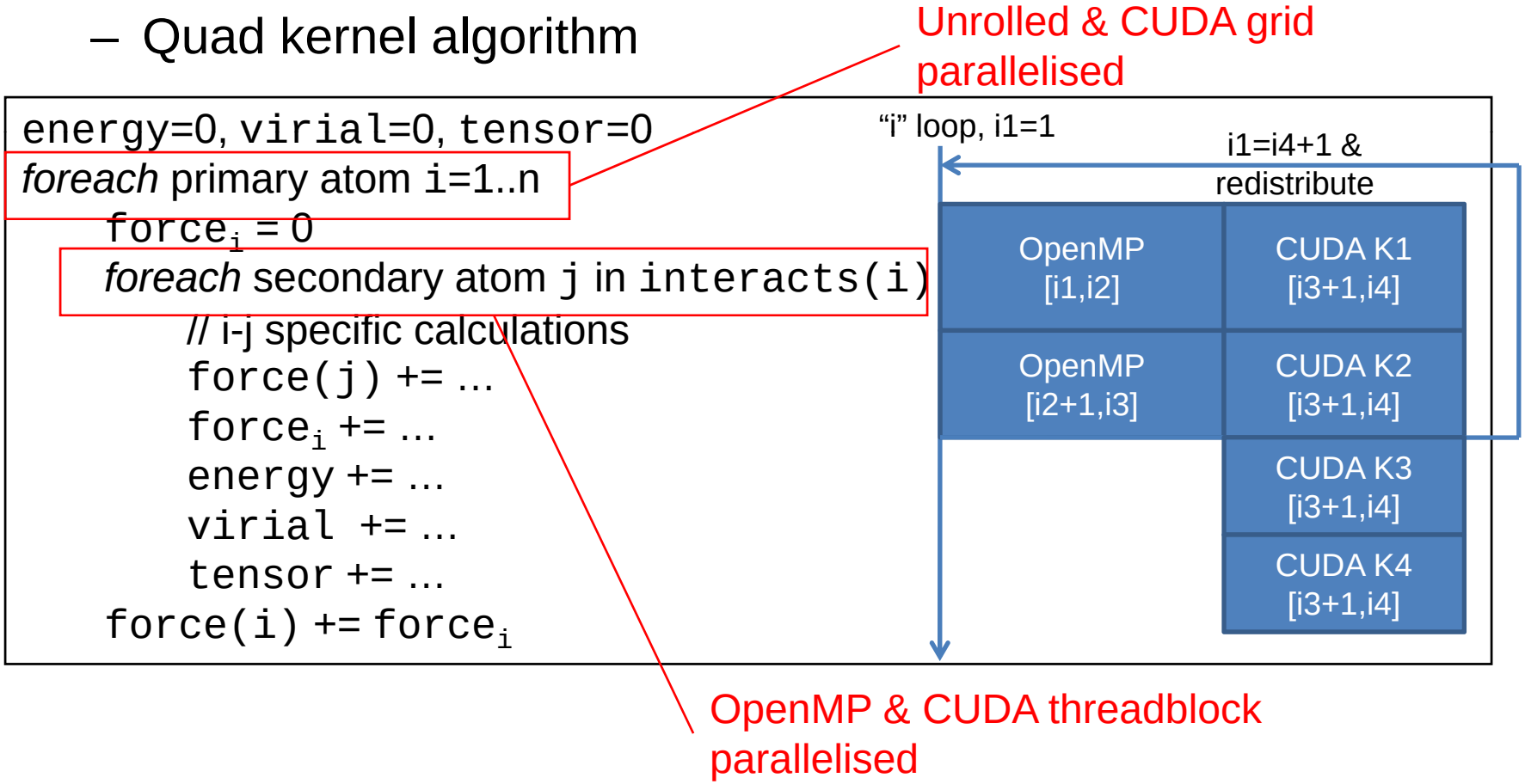
- Pair-wise calculations
  - `interacts(i)` is the atoms that atom "`i`" interacts with ("link cells" algorithm).

```
energy=0, virial=0, tensor=0
foreach primary atom i=1..n
    force_i = 0
    foreach secondary atom j in interacts(i)
        // i-j specific calculations
        force(j) += ...
        force_i += ...
        energy += ...
        virial += ...
        tensor += ...
    force(i) += force_i
```

loop-carried dependencies

Two-Body Force Field Algorithm (2)

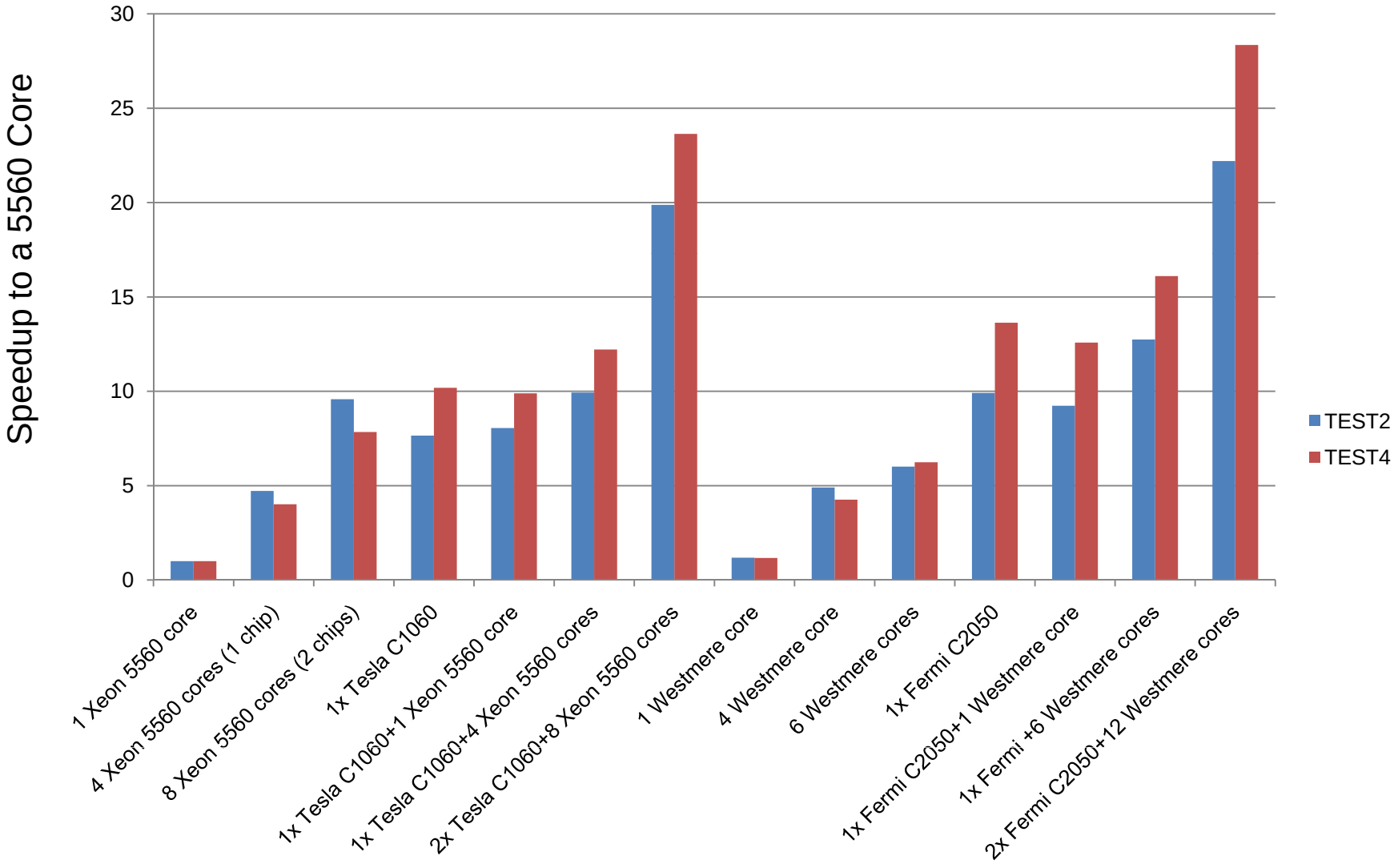
- OpenMP targets the secondary atoms loop.
- CUDA targets both loops for 10000s of threads.
  - Quad kernel algorithm



Performance (1)

- Configuration
  - Intel Nehalem (Xeon 5560) & Intel Westmere.
  - Tesla (C1060), Fermi (S2050).
  - Speedup versus a single 5560 core (11.2GFLOPs)
- Test cases
  - TEST2: Sodium Chloride, 216000 Ions.
  - TEST4: DMPC in Water, 413896 Atoms.
- Double precision only.

Performance (2)



Performance (3)

- Average speedup (idle host)
  - 1 Tesla C1060 ~= 8.19 Xeon 5560 cores
  - 1 Fermi S2050 ~= 11.77 Xeon 5560 cores.
- Fermi reduced time by ~30%
  - Pairwise calculations heavily memory-bound.
  - C2050 has 140GB/sec, C1060 has 102GB/sec, i.e. a 27% improvement.
- Fermi's multi-context support.