Implementation of NAMD molecular dynamics non-bonded force-field on the Cell Broadband Engine processor

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Cell Processor and IBM Cell Blade

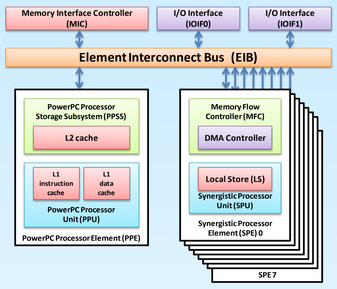


Figure 1: Cell/B.E. processor architecture

- One Power Processor Element (PPE) and eight Synergistic Processing Elements (SPEs)
- SPE's local storage (LS): 256 KB Processor clock speed: 3.2 GHz
- 25.6 GB/s processor-to-memory bandwidth
- 205 GB/s EIB sustained aggregate bandwidth
- Theoretical peak performance: 204.8 GFLOPS (SP) and 14.63 GFLOPS (DP)

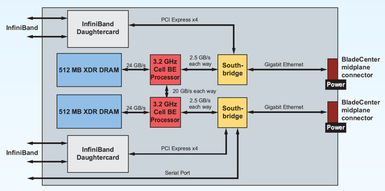


Figure 2: IBM dual-Cell/B.E. blade

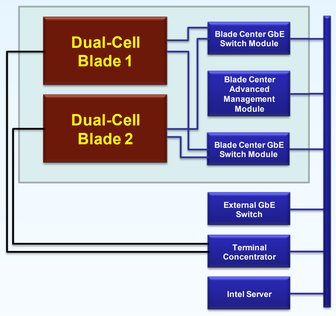


Figure 3: IBM Cell/B.E. blade center

- 410/28 GFLOPS (SP/DP) peak
- 512 MB of XDR DRAM per Cell/B.E. processor
- Gigabit Ethernet

Function offload programming model

- User compute task structure inherits the common *task_t* structure:

```
typedef struct task_s {
      int cmd; // operand
      int size; // size of task structure
} task_t;
```

```
typedef struct compute_task_s {
      task_t common;
       <user_type1> <user_var_name1>
       <user_type2> <user_var_name2>
        …
} compute_task_t;
```

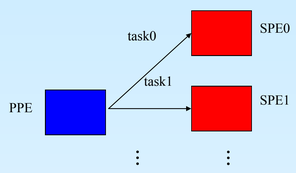


Figure 4: Task based function offload model

- API for the PPE

```
int ppu_task_init(int argc, char **argv,spe_program_handle_t );  // initialization
int ppu_task_run(volatile task_t * task);  // start a task in all SPEs
int ppu_task_spu_run(volatile task_t* task, int spe); // start a task in one SPE
int ppu_task_spu_wait(void); // wait for any SPE to finish, blocking call
void ppu_task_spu_waitall(void); // wait for all SPEs to finish, blocking call
```

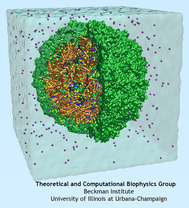
- API for the SPEs

```
int spu_task_init(unsigned long long);
int spu_task_register(dotask_t,int);  // register a task
int spu_task_run(void);  // start the infinite loop, wait for tasks
```

- Two programming models are supported: *single SPE* and *multiple SPEs*

NAMD kernel

NAMD is a parallel molecular dynamics code designed for high-performance simulation of large biomolecular systems.



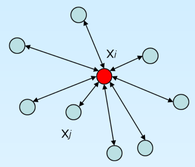
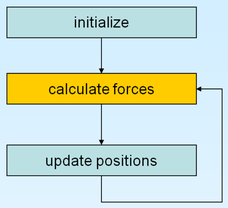


Figure 5: MD simulation principles



x_i^k — time step; atom index

$$F(x_i^k) := \sum_{i \neq j=1}^{N} f(x_i^k, x_j^k)$$

$$x_i^{k+1} = x_i^k + f(F(x_i^k))$$

NAMD SPEC 2006 CPU benchmark kernel:

```
1: for each atom i in patch p_k
2:       for each atom j in patch p_l
3:             if atoms i and j are bonded, compute bonded forces
4:             otherwise, if atoms i and j are within the cutoff distance, add atom j to the i's atom pair list
5:       end
6:       for each atom k in the i's atom pair list
7:             compute non-bonded forces (L-J potential and PME direct sum, both vial lookup tables)
8:       end
```

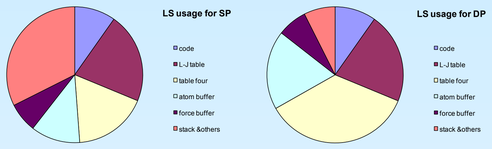
We implemented a simplified version of the kernel that excludes pairlists and bonded forces:

```
1: for each atom i in patch p_k
2:       for each atom j in patch p_l
3:             if atoms i and j are within the cutoff distance
4:                   compute non-bonded forces (L-J potential and PME direct sum, both via lookup tables)
5:       end
6: end
```

SPU NAMD Kernel implementation

Kernel type	*Code*	*L-J table*	*table_four*	*atom buffer*	*force buffer*	*stack & other*
single-precision	25KB	55KB	45KB	30KB	18KB	83KB
double-precision	25KB	55KB	91KB	48KB	18KB	19KB

Table 1: SPE LS memory usage for different kernel types



- Entire patch is loaded into SPE's local storage
- Double-precision case just fits, single-precision still have some space left
- Substantial number of data movement operations are needed

```
vector float * m = (vector float*) pj;
vector float x,y,z,c, delta_x, delta_y, delta_z, r2;

{
     vector float v1, v2, v3, v4, v5, v6, v7, v8, v9;

     v1 = spu_shuffle(*m, *(m+1), ptn1);

     v2 = spu_shuffle(*m, *(m+1), ptn2);
     v3 = spu_shuffle(*(m+2), *(m+3), ptn3);
     v4 = spu_shuffle(*(m+2), *(m+3), ptn4);
     v5 = spu_shuffle(v4, *(m+4), ptn5);
     v6 = spu_shuffle(v4, *(m+4), ptn6);
     v7 = spu_shuffle(v1, v3, ptn7);
     v8 = spu_shuffle(v1, v3, ptn8);
     v9 = spu_shuffle(v2, v3, ptn9);

     x = v7;
     y = spu_shuffle(v5,v8, ptn_y);
     z = spu_shuffle(v5,v2, ptn_z);
     c = spu_shuffle(v9,v6, ptn_c);
   }


   delta_x = spu_sub(ix, x);
   delta_y = spu_sub(iy, y);
   delta_z = spu_sub(iz, z);

   r2 = spu_madd(delta_x, delta_x, r2);
   r2 = spu_madd(delta_y, delta_y, r2);
   r2 = spu_madd(delta_z, delta_z, r2);
    ....
```

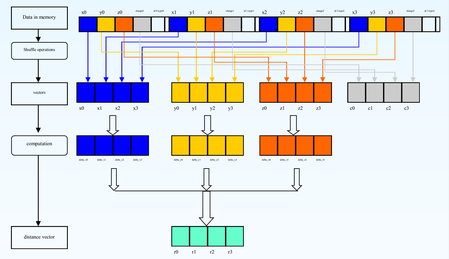


Figure 6: Data movement for distance computation (SP case)

NAMD on Cell: program flow

Different vectorization schemes are applied in order to get best performance:

- **Self-compute**: fill zeros in unused slots
- **Pair-compute**: save enough pairs of atoms, then do calculations

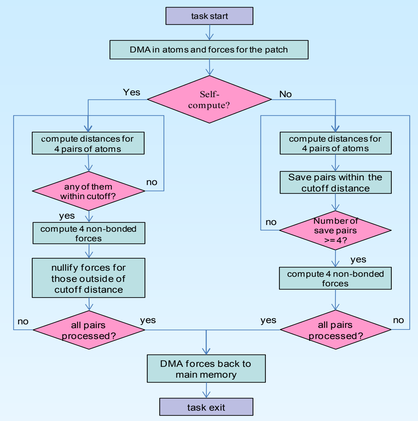


Figure 7: SPE Program flow

PPE runs a task dispatch system:

- Find dependency-free task
- Schedule the task on the idle SPE

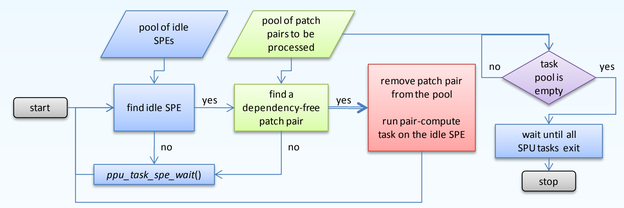


Figure 8: Task dispatch system running on the PPE

Performance

- Distance computation code takes most of the execution time
- Data manipulation time is significant

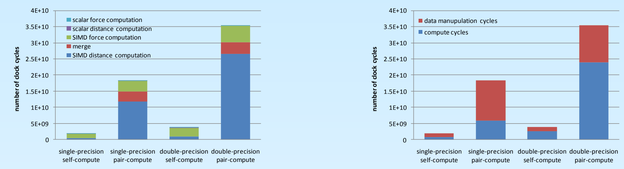


Figure 9: Static analysis of the computing kernels performed with the help of the timing tool, spu_timing

- Perfect scaling on multiple SPEs
- >10x speedup compared with Intel Xeon processor

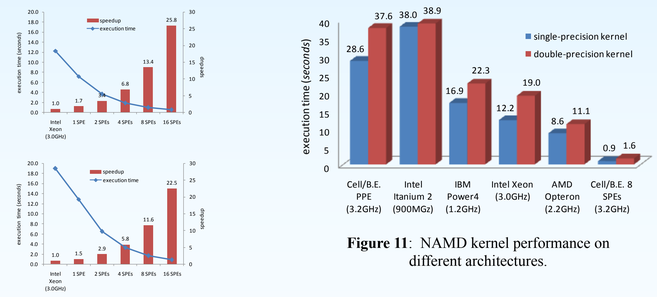


Figure 11: NAMD kernel performance on different architectures.

Figure 10: Scaling and speedup of the force-field kernel implementation as compared to a 3.0 GHz Intel Xeon processor.

Acknowledgements

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