



# PROGRAMMING AND OPTIMIZATION FOR INTEL<sup>®</sup> ARCHITECTURE

Hands-On Workshop (HOW) Series "Deep Dive"  
Session 6

*Colfax International* — [colfaxresearch.com](http://colfaxresearch.com)

April 2017

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- ▶ **Module I. Programming**
  - 01. Intel Architecture and Modern Code – Apr 17
  - 02. Xeon Phi, Coprocessors, Omni-Path – Apr 18
- ▶ **Module II. Expressing Parallelism**
  - 03. Automatic vectorization – Apr 19
  - 04. Multi-threading with OpenMP – Apr 20
  - 05. Distributed Computing, MPI – Apr 21
- ▶ **Module III. Optimization**
  - 06. Optimization Overview: N-body – Apr 24
  - 07. Scalar tuning, Vectorization – Apr 25
  - 08. Common Multi-threading Problems – Apr 26
  - 09. Multi-threading, Memory Aspect – Apr 27
  - 10. Access to Caches and Memory – Apr 28

April 2017						
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■ — Webinar+remote access

Course page:

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- ▶ Slides
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**Forum**

**Colfax Cluster**  
Discussion of Colfax Cluster usage policies, troubleshooting.

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Questions about any of the Colfax trainings? Usage of training servers, experience with specific exercises, inquiries on what's inside, suggestions for future trainings - post them here.

**Performance Optimization and Parallelism**  
Discuss with Colfax Research and colleagues any topics related to computational science, parallel programming, performance optimization and code modernization.

[colfaxresearch.com/discussion](https://colfaxresearch.com/discussion)

- ▶ All registrants receive an invitation from `cluster@colfaxresearch.com`
- ▶ Queue-based access to Intel Xeon E5, Intel Xeon Phi (KNC and KNL)
- ▶ Can access the cluster the entire 2 weeks of the workshop





## **§2. PERFORMANCE OPTIMIZATION**

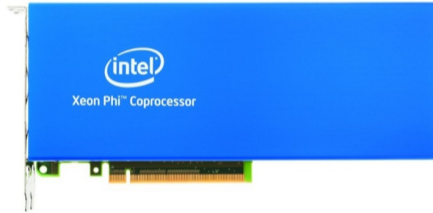
## Intel Xeon Processor



Current: Broadwell  
Upcoming: Skylake

Multi-Core Architecture

## Intel Xeon Phi Coprocessor, 1st generation



Knights Corner (KNC)

## Intel Xeon Phi Processor, 2nd generation\*

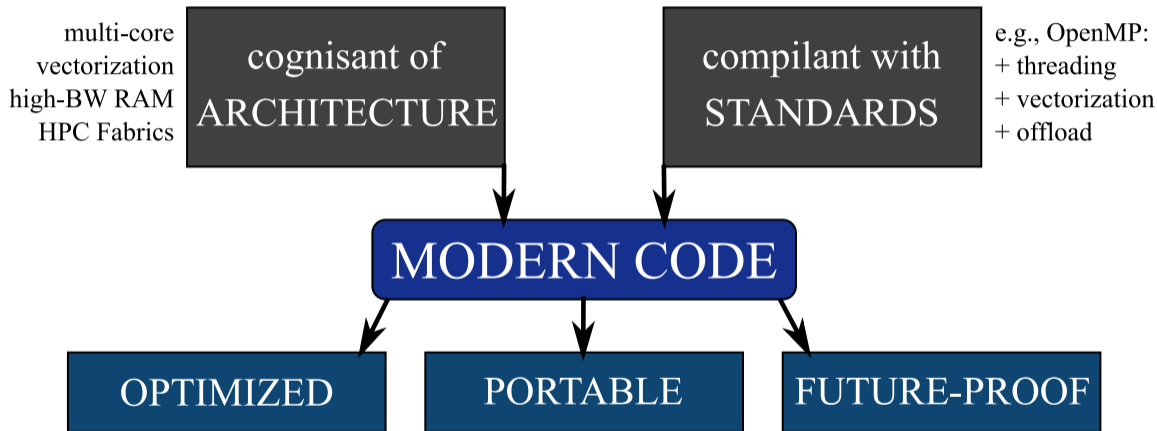


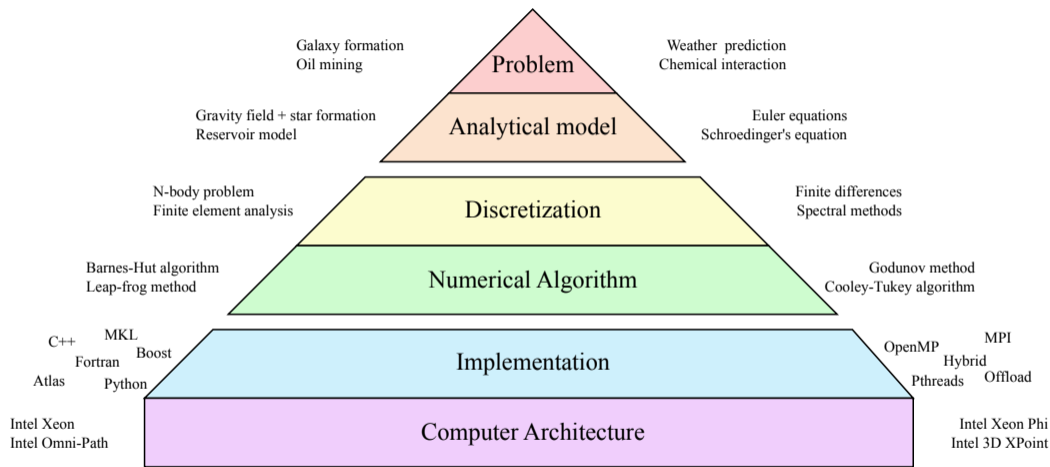
\* socket and coprocessor versions

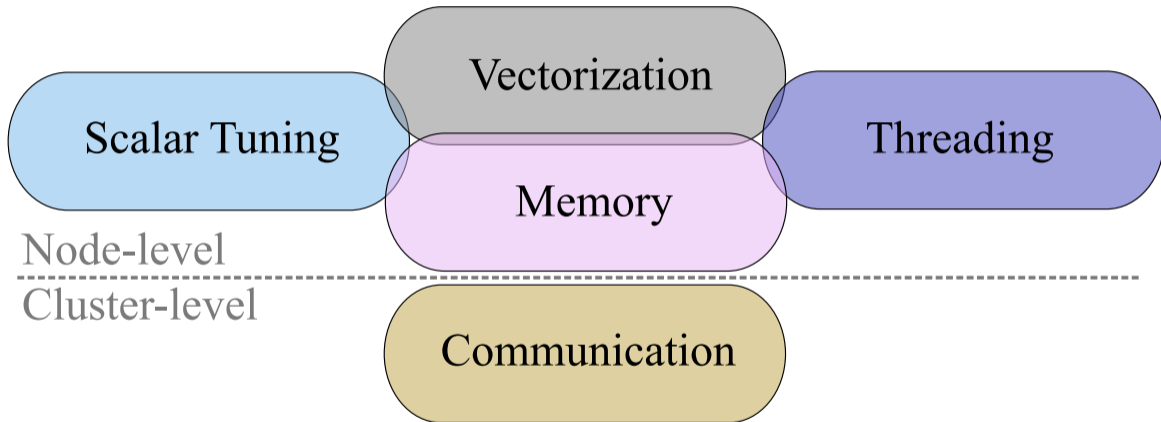
Knights Landing (KNL)

Intel Many Integrated Core (MIC) Architecture

# ONE CODE FOR ALL PLATFORMS

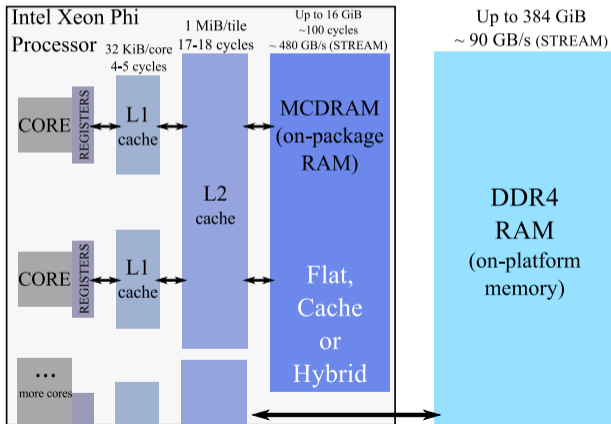






# KNL MEMORY ORGANIZATION (BOOTABLE)

- ▶ On-package high-bandwidth memory (HBM) – MCDRAM
- ▶ Optimized for arithmetic performance and bandwidth (not latency)



## **§3. N-BODY SIMULATION**



# PHYSICS

# N-BODY SIMULATION ON CPU AND COPROCESSOR



## N-body simulation on...

Two  
Intel® Xeon®  
CPUs



One  
Intel® Xeon Phi™  
coprocessor



Two  
Intel® Xeon Phi™  
coprocessors



Paper: <http://xeonphi.com/papers/nbody-basic>

Demo: [click here](#)

## Gravitational N-body dynamics:

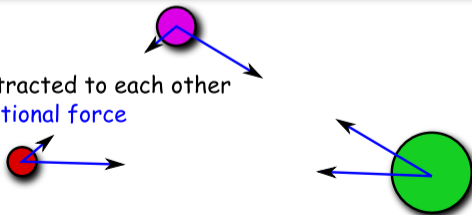
Newton's law of universal gravitation:

$$M_i \vec{R}_i''(t) = G \sum_j \frac{M_i M_j}{|\vec{R}_i - \vec{R}_j|^3} (\vec{R}_j - \vec{R}_i)$$

where:

$$|\vec{R}_i - \vec{R}_j| = \sqrt{(R_{i,x} - R_{j,x})^2 + (R_{i,y} - R_{j,y})^2 + (R_{i,z} - R_{j,z})^2}$$

particles are attracted to each other  
with the gravitational force



# APPLICATION

## 1. Astrophysics:

- planetary systems
- galaxies
- cosmological structures

## 2. Electrostatic systems:

- molecules
- crystals

This work: “toy model” with all-to-all  $O(n^2)$  algorithm. Practical N-body simulations may use tree algorithms with  $O(n \log n)$  complexity.



Source: [APOD](#), credit: Debra Meloy Elmegreen (Vassar College) et al., & the Hubble Heritage Team (AURA/ STScI/ NASA)

# ALL-TO-ALL APPROACH ( $O(n^2)$ COMPLEXITY SCALING)

Each particle is stored as a structure:

```
1 struct ParticleType {  
2     float x, y, z;  
3     float vx, vy, vz;  
4 };
```

main() allocates an array of ParticleType:

```
1 ParticleType* particle = new ParticleType[nParticles];
```

Particle propagation step is timed:

```
1 const double tStart = omp_get_wtime(); // Start timing  
2 MoveParticles(nParticles, particle, dt);  
3 const double tEnd = omp_get_wtime(); // End timing
```



# OPTIMIZATION

# PARTICLE UPDATE ENGINE

```
1 void MoveParticles(int nParticles, ParticleType* particle, float dt) {
2     for (int i = 0; i < nParticles; i++) { // Particles that experience force
3         float Fx = 0, Fy = 0, Fz = 0; // Gravity force on particle i
4         for (int j = 0; j < nParticles; j++) { // Particles that exert force
5             // Newton's law of universal gravity
6             const float dx = particle[j].x - particle[i].x;
7             const float dy = particle[j].y - particle[i].y;
8             const float dz = particle[j].z - particle[i].z;
9             const float drSquared = dx*dx + dy*dy + dz*dz + 1e-20;
10            const float drPower32 = pow(drSquared, 3.0/2.0);
11            // Calculate the net force
12            Fx += dx/drPower32; Fy += dy/drPower32; Fz += dz/drPower32;
13        }
14        // Accelerate particles in response to the gravitational force
15        particle[i].vx+=dt*Fx; particle[i].vy+=dt*Fy; particle[i].vz+=dt*Fz;
16    }
```

# INCORPORATING THREAD PARALLELISM

Before:

```
1  for (int i = 0; i < nParticles; i++) { // Particles that experience force
2      float Fx = 0, Fy = 0, Fz = 0; // Gravity force on particle i
3      for (int j = 0; j < nParticles; j++) { // Particles that exert force
4          // Newton's law of universal gravity
5          ...
```

After:

```
1  #pragma omp parallel for
2      for (int i = 0; i < nParticles; i++) { // Particles that experience force
3          float Fx = 0, Fy = 0, Fz = 0; // Gravity force on particle i
4          for (int j = 0; j < nParticles; j++) { // Particles that exert force
5              // Newton's law of universal gravity
6              ...
```

# IMPROVING SCALAR EXPRESSIONS

Before:

```
1  const float drSquared  = dx*dx + dy*dy + dz*dz + 1e-20;  
2  const float drPower32 = pow(drSquared, 3.0/2.0);  
3  // Calculate the net force  
4  Fx += dx/drPower32;  Fy += dy/drPower32;  Fz += dz/drPower32;
```

After:

```
1  const float drRecip    = 1.0f/sqrtf(dx*dx + dy*dy + dz*dz + 1e-20);  
2  const float drPowerN32 = drRecip*drRecip*drRecip;  
3  // Calculate the net force  
4  Fx += dx*drPowerN32;  Fy += dy*drPowerN32;  Fz += dz*drPowerN32;
```

- ▶ Strength reduction (division → multiplication by reciprocal)
- ▶ Precision control (suffix `-f` on single-precision constants and functions)
- ▶ Reliance on hardware-supported reciprocal square root

# VECTORIZING WITH UNIT-STRIDE MEMORY ACCESS

Before:

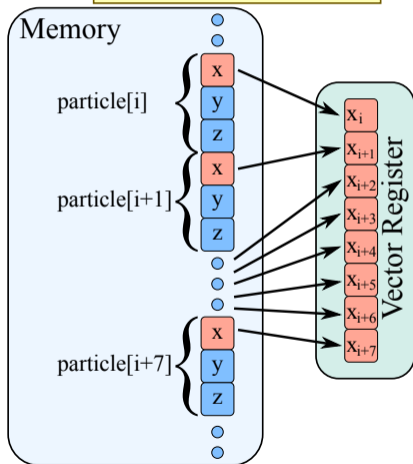
```
1 struct ParticleType {  
2     float x, y, z, vx, vy, vz;  
3 }; // ...  
4     const float dx = particle[j].x - particle[i].x;  
5     const float dy = particle[j].y - particle[i].y;  
6     const float dz = particle[j].z - particle[i].z;
```

After:

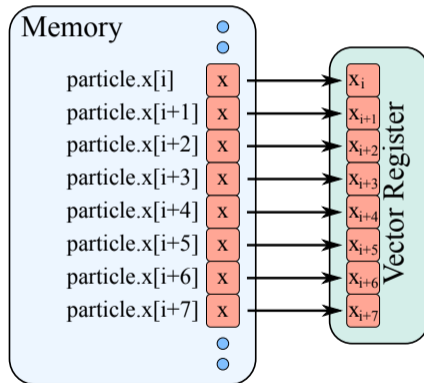
```
1 struct ParticleSet {  
2     float *x, *y, *z, *vx, *vy, *vz;  
3 }; // ...  
4     const float dx = particle.x[j] - particle.x[i];  
5     const float dy = particle.y[j] - particle.y[i];  
6     const float dz = particle.z[j] - particle.z[i];
```

# WHY AOS TO SOA CONVERSION HELPS: UNIT STRIDE

Array of Structures  
(sub-optimal)



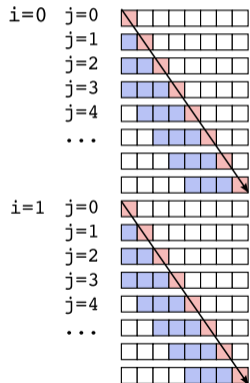
Structure of Arrays  
(optimal)



# LOOP TILING: REGISTER BLOCKING

## Original:

```
for (i=0; i<m; i++)
  for (j=0; j<n; j++)
    ...=*b[j];
```



- - cached, LRU eviction policy
- - cache miss (read from memory, slow)
- - cache hit (read from cache, fast)

Cache size: 4

TILE=4

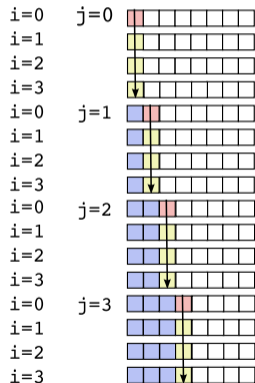
(must be tuned to cache size)

Cache hit rate without tiling: 0%

Cache hit rate with tiling: 50%

## Tiled:

```
for (ii=0; ii<m; ii+=TILE)
  for (j=0; j<n; j++)
    for (i=ii; i<ii+TILE; i++)
      ...=*b[j];
```



# IMPROVING CACHE TRAFFIC

Before:

```

1  for (int i = 0; i < nParticles; i++) { // Particles that experience force
2      float Fx = 0, Fy = 0, Fz = 0; // Gravity force on particle i
3      for (int j = 0; j < nParticles; j++) { // Particles that exert force
4          // ...
5          Fx += dx*drPowerN32; Fy += dy*drPowerN32; Fz += dz*drPowerN32;

```

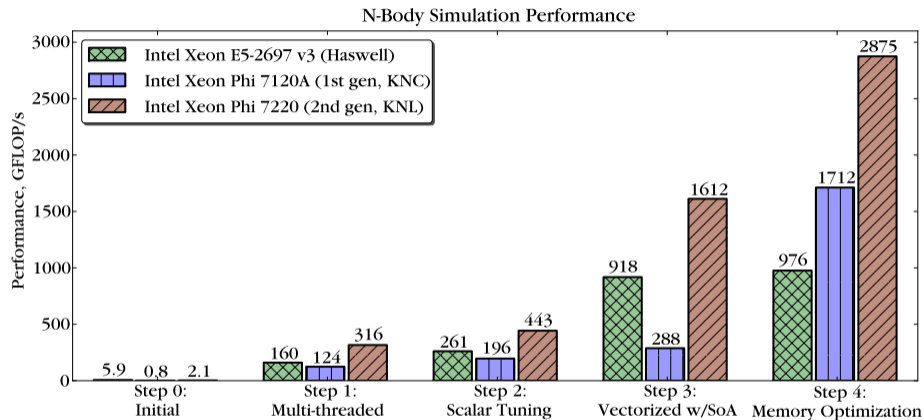
After: (tileSize = 16)

```

1  for (int ii = 0; ii < nParticles; ii += tileSize) { // Particle blocks
2      float Fx[tileSize], Fy[tileSize], Fz[tileSize]; // Force on particle block
3      Fx[:] = Fy[:] = Fz[:] = 0;
4      #pragma unroll(tileSize)
5      for (int j = 0; j < nParticles; j++) { // Particles that exert force
6          for (int i = ii; i < ii + tileSize; i++) { // Traverse the block
7              // ...
8              Fx[i-ii] += dx*drPowerN32; Fy[i-ii] += dy*drPowerN32; Fz[i-ii] += dz*drPowerN32;

```

# IMPACT OF CODE OPTIMIZATION



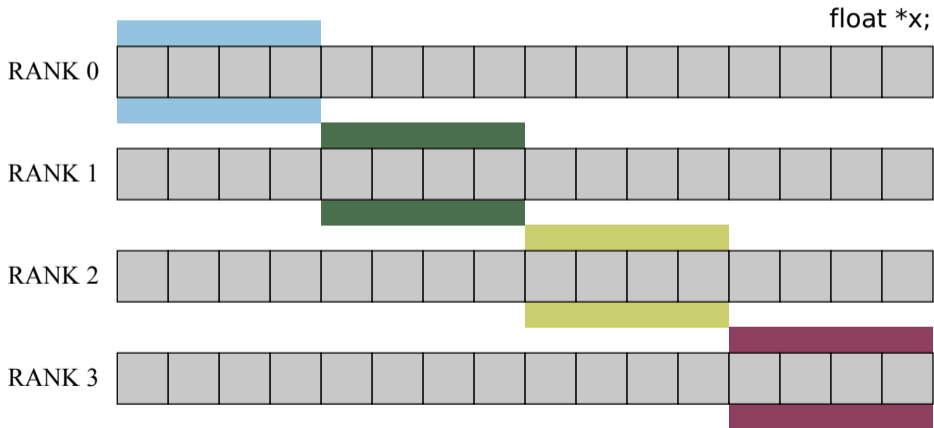
Contributed as Chapter 23 in “[Intel Xeon Phi Processor High Performance Programming, Knights Landing Edition](#)” (2016)



# **MPI IMPLEMENTATION**

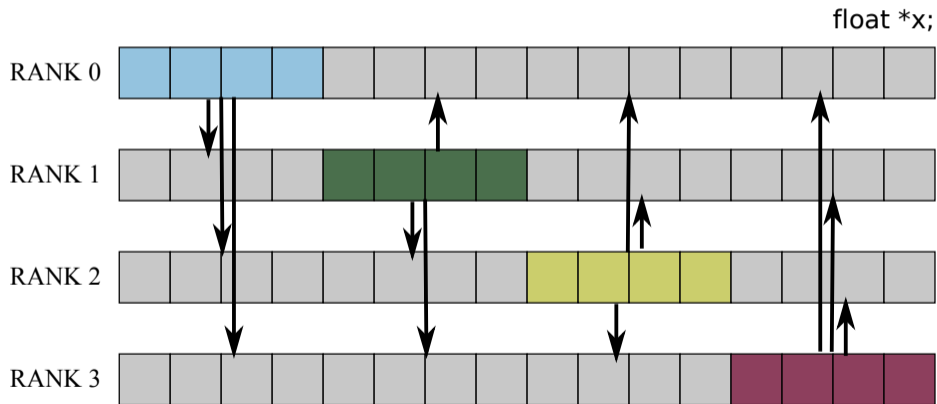
# WORK DISTRIBUTION

- ▶ All processes start with same complete set of particle coordinates.
- ▶ Each processor moves only its share of particles



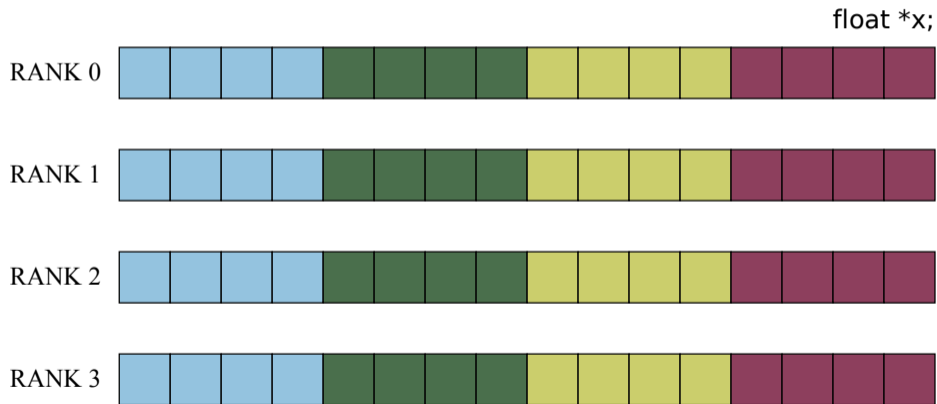
# COMMUNICATION

- ▶ After time step, need to propagate modified particles to all peers
- ▶ Use the Allgather operation from MPI



# COMMUNICATION

- ▶ All processors end up with the same data set again
- ▶ Only  $x$ ,  $y$ ,  $z$  need to be propagated.  $v_x$ ,  $v_y$ ,  $v_z$  stay local



# CORE OF MPI-ONLY IMPLEMENTATION

Simple: all particles on each compute node; exchange updated particle coordinates.

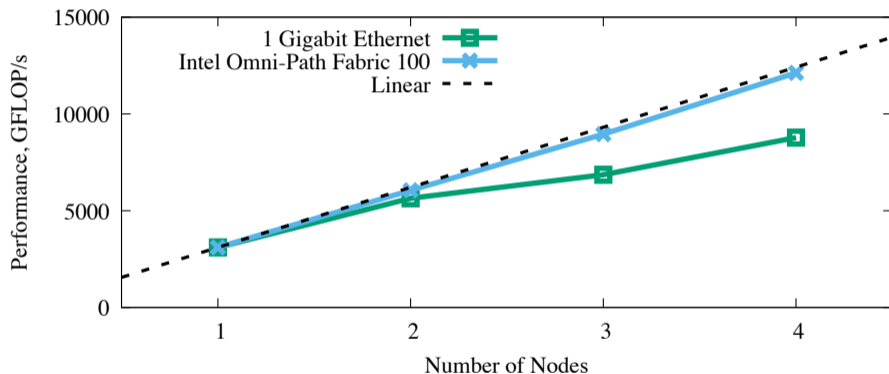
```

1 void MoveParticles(int nParticles, ParticleSet& particle, float dt,
2                   int mpiRank, int mpiWorldSize) {
3     const int myParticles = nParticles/mpiWorldSize;
4     const int startParticle = (mpiRank    )*myParticles;
5     const int endParticle   = (mpiRank + 1)*myParticles;
6     // Outer loop over only the subset of particles processed by present process
7     #pragma omp parallel for schedule(guided)
8     for (int ii = startParticle; ii < endParticle; ii += tileSize) {
9         for (int j = 0; j < nParticles; j++) // ...But inner loop over all particles
10            //...
11    }
12    // ... Propagate results of time step across the cluster
13    MPI_Allgather(MPI_IN_PLACE, 0, MPI_DATATYPE_NULL, particle.x,
14                 myParticles, MPI_FLOAT, MPI_COMM_WORLD);
15    // ...

```

# PERFORMANCE WITH MPI

Intel Xeon Phi 7210 processors,  $N = 2^{18}$  particles



Impact of communication decreases with increasing  $N$ .

Areas of optimization of applications for Intel Xeon and Intel Xeon Phi processors:

1. **Scalar optimization** (compiler-friendly practices)
2. **Vectorization** (must use 16- or 8-wide vectors)
3. **Multi-threading** (must scale to 100+ threads)
4. **Memory access** (streaming access or tiling)
5. **Communication** (offload, MPI traffic control)

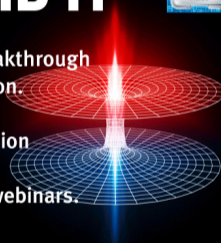
Next session: scalar tuning, optimization of vectorization.

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