PROGRAMMING AND OPTIMIZATION FOR INTEL® ARCHITECTURE

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

Session 6

Colfax International — *colfaxresearch.com*

February 2017

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COURSE ROADMAP

- Module I. Programming
  - 01. Intel Architecture and Modern Code – Feb 13
  - 02. Xeon Phi, Coprocessors, Omni-Path – Feb 14
- Module II. Expressing Parallelism
  - 03. Automatic vectorization – Feb 15
  - 04. Multi-threading with OpenMP – Feb 16
  - 06. Distributed Computing, MPI – Feb 17
- Module III. Optimization
  - 06. Optimization Overview: N-body – Feb 20
  - 07. Scalar tuning, Vectorization – Feb 21
  - 08. Common Multi-threading Problems – Feb 22
  - 09. Multi-threading, Memory Aspect – Feb 23
  - 10. Access to Caches and Memory – Feb 24

February 2017

S	M	T	W	H	F	S
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12	13	14	15	16	17	18
19	20	21	22	23	24	25
26	27	28				

— Webinar+remote access

HOW SERIES ONLINE

Course page:
colfaxresearch.com/how-17-02

- Slides
- Code
- Video
- Chat

More workshops:
colfaxresearch.com/training

GET YOUR QUESTIONS ANSWERED: CHAT

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Forum

Colfax Cluster

Discussion of Colfax Cluster usage policies, troubleshooting.

Modern Code

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

Developer Training

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.

Colfax News

Subscribe to this forum is you wish to receive updates on new papers, training events, and other news we may have. Updates here are frequent and

colfaxresearch.com/discussion

HANDS-ON EXERCISES AND REMOTE ACCESS

- 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

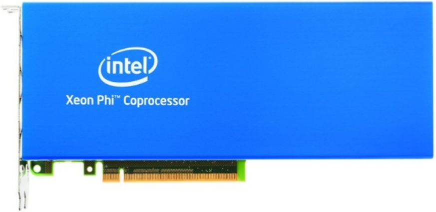
§2. PERFORMANCE OPTIMIZATION

COMPUTING PLATFORMS

Intel Xeon Processor

Current: Broadwell
Upcoming: Skylake

Intel Xeon Phi Coprocessor, 1st generation



Knights Corner (KNC)

Intel Xeon Phi Processor, 2nd generation*

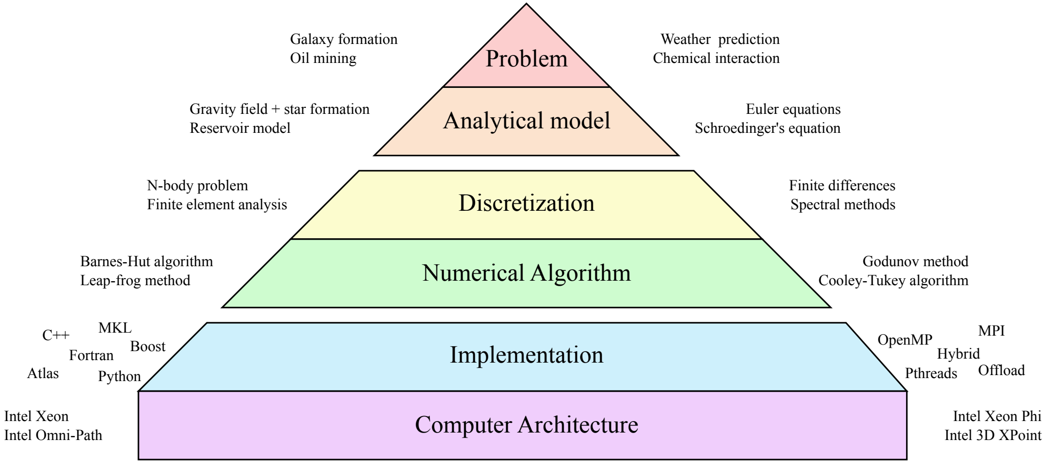
* socket and coprocessor versions

Knights Landing (KNL)

Multi-Core Architecture

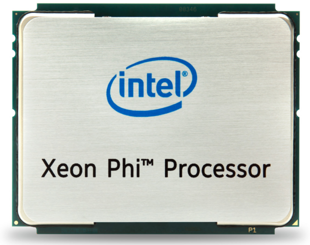
Intel Many Integrated Core (MIC) Architecture

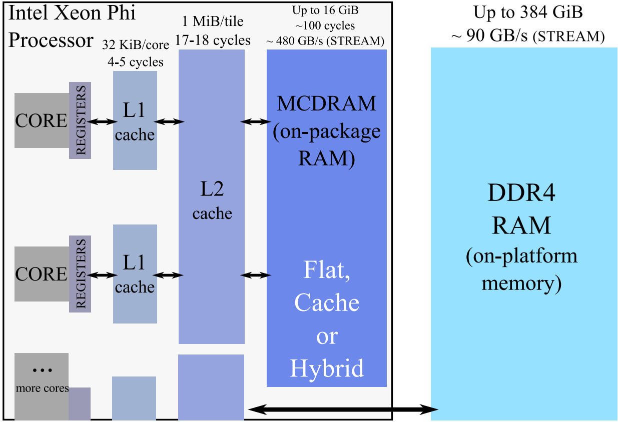
COMPUTING IN SCIENCE AND ENGINEERING



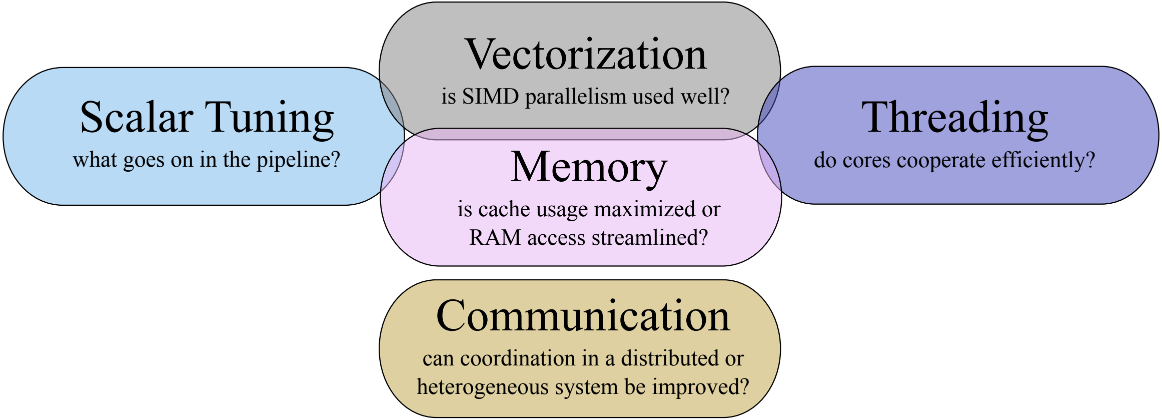
KNL MEMORY ORGANIZATION (BOOTABLE)

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





OPTIMIZATION AREAS



§3. N-BODY SIMULATION

PHYSICS

N-BODY SIMULATION ON CPU AND COPROCESSOR

COLFAX
Customized Solutions

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:

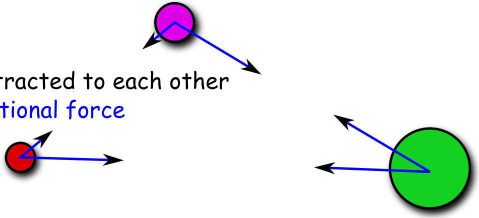
Newton's law of universal gravitation:

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

where:

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

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:

```
struct ParticleType {
  float x, y, z;
  float vx, vy, vz;
};
```

main() allocates an array of ParticleType:

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

Particle propagation step is timed:

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

OPTIMIZATION

PARTICLE UPDATE ENGINE

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


INCORPORATING THREAD PARALLELISM

Before:

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

After:

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

IMPROVING SCALAR EXPRESSIONS

Before:

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

After:

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

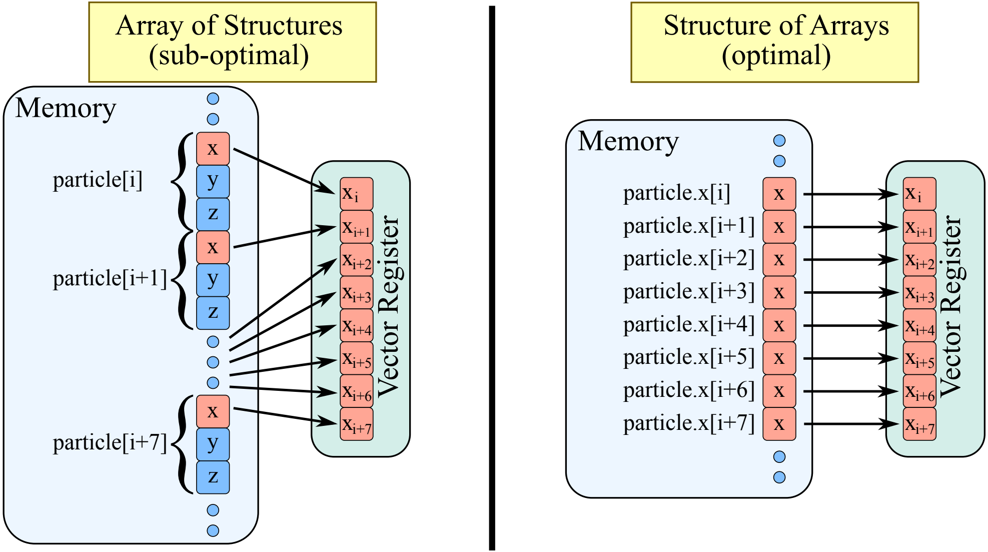
Before:

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

After:

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

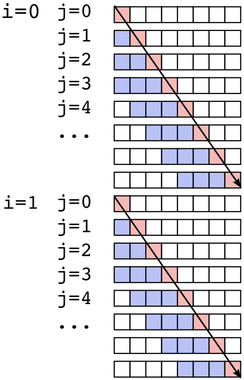
WHY AOS TO SOA CONVERSION HELPS: UNIT STRIDE



LOOP TILING

Original:

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



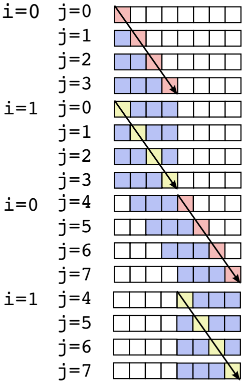
- cached, LRU eviction policy
- cache miss (read from memory, slow)
- cache hit (read from cache, fast)

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



IMPROVING CACHE TRAFFIC

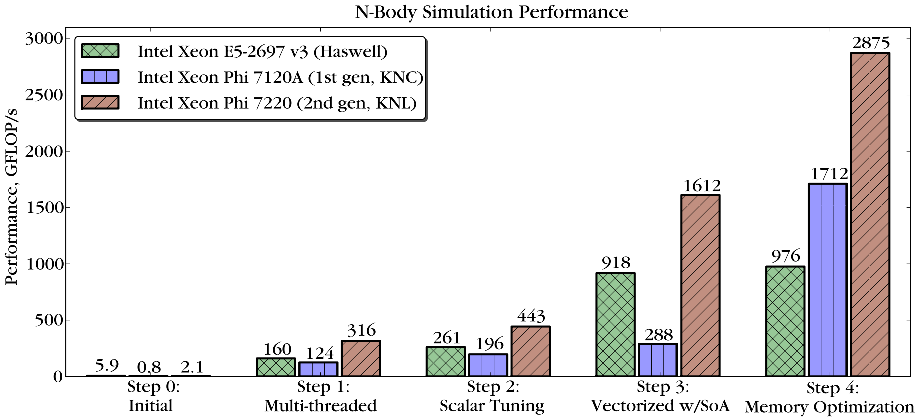
Before:

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

After: (`tileSize = 16`)

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

IMPACT OF CODE OPTIMIZATION

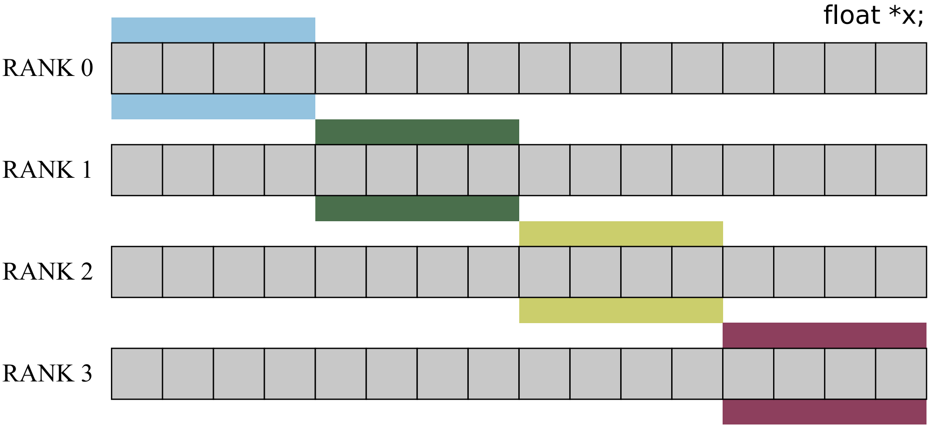


Contributed as Chapter 23 in “Intel Xeon Phi Processor High Performance Programming, Knights Landing Edition” (2016)

MPI IMPLEMENTATION

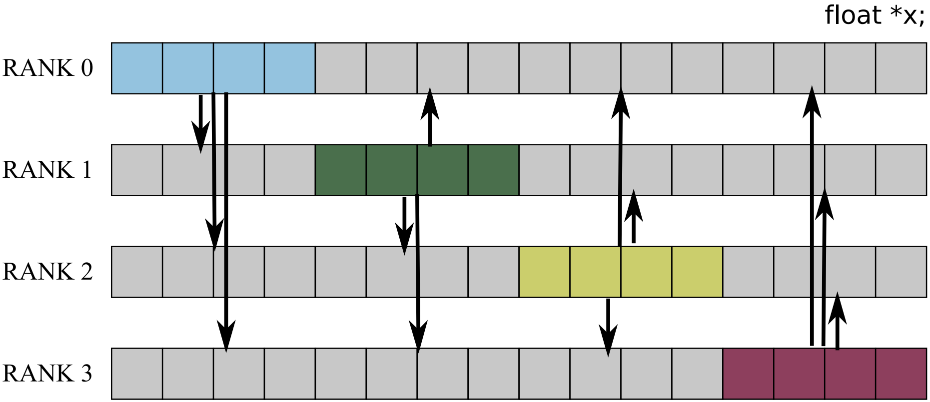
WORK DISTRIBUTION

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



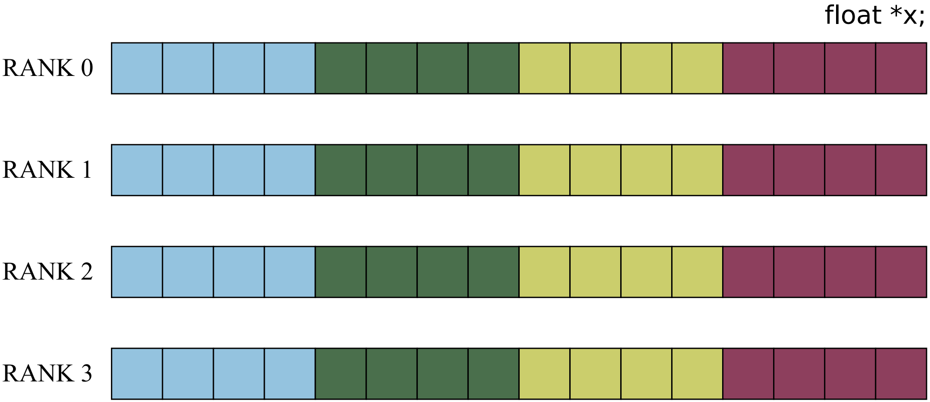
COMMUNICATION

- 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. vx, vy, vz stay local



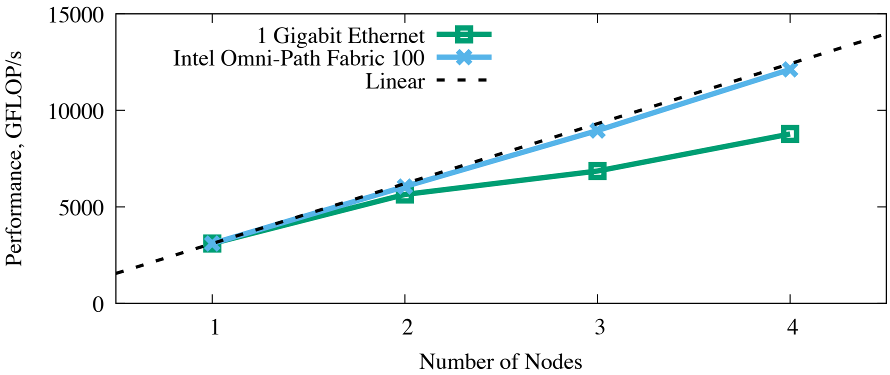
CORE OF MPI-ONLY IMPLEMENTATION

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

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

Performance with MPI

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



Impact of communication decreases with increasing N.

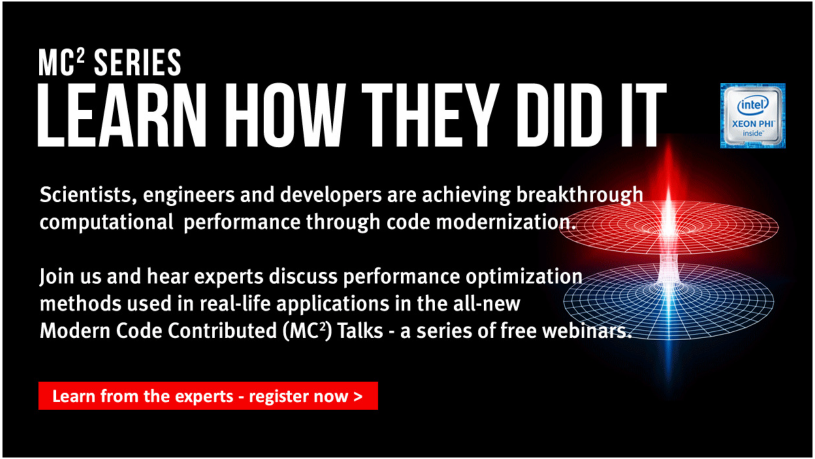
Summary

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)

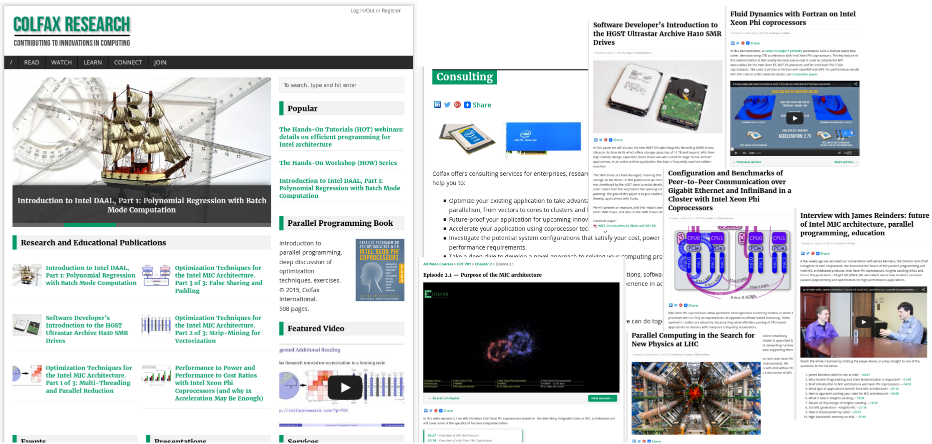
Next session: scalar tuning, optimization of vectorization.

NEW PROJECT: MC^2 SERIES



mc2series.com

COLFAX RESEARCH



http://colfaxresearch.com/