Hotspot-Guided Optimization with Intel VTune Amplifier XE

The Hands-On Workshop (HOW) Series "Tools"

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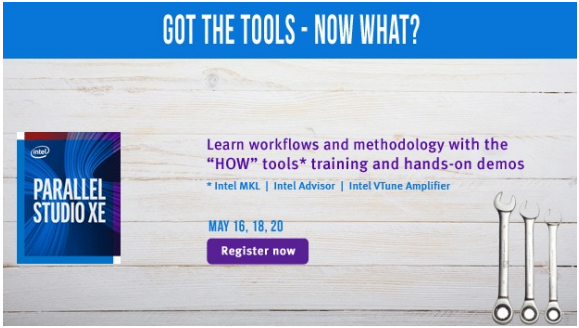
About the Series

Hands-On Workshop (HOW “Tools” Series): webinars on efficient programming for the Intel architecture with the help of dedicated software development tools



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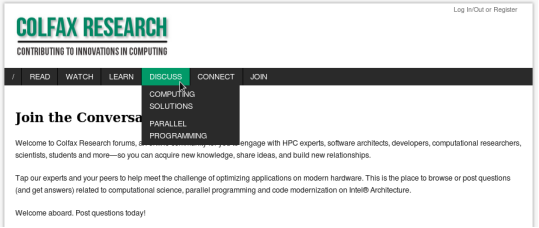


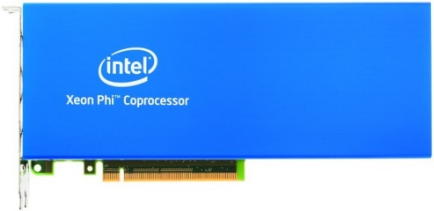
§2. Intel Architecture

Computing Platforms

Intel Xeon Processor

Current: Broadwell
Upcoming: Skylake

Intel Xeon Phi Coprocessor, 1st generation



Current: Knights Corner (KNC)

Intel Xeon Phi Processor, 2nd generation*

* socket and coprocessor versions

Upcoming: Knights Landing (KNL)

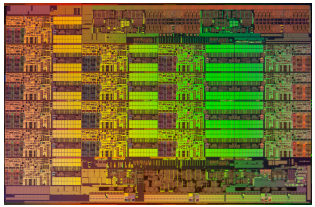
Multi-Core Architecture

Intel Many Integrated Core (MIC) Architecture

Intel Xeon CPU: Purpose and Specifications

General-purpose platform for demanding computing applications.

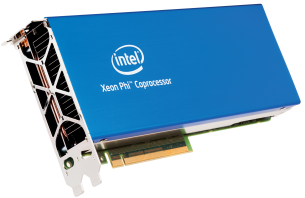
- Up to ~ 1 TFLOP/s in DP
- Up to ~ 2 TFLOP/s in SP
- Up to 768 GiB DDR4 RAM
- ~ 126 GB/s bandwidth
- Hardware-rich: forgiving of sub-optimal code

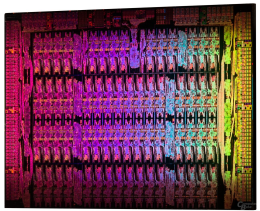


Intel Xeon Phi Processors (1st Gen)

Specialized platform for demanding computing applications.

- PCIe end-point device
- ~ 1.2 TFLOP/s in DP
- ~ 2.4 TFLOP/s in SP
- Up to 16 GiB GDDR5 RAM
- ~ 176 GB/s bandwidth
- Heterogeneous clustering
- Runs special Linux distribution

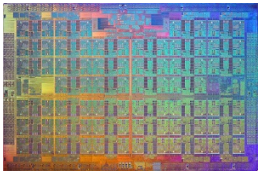




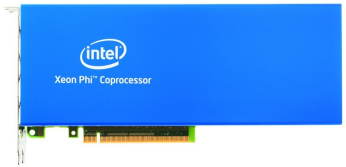
Intel Xeon Phi Processors (2nd Gen)

Specialized platform for demanding computing applications.

- Socket version or coprocessor
- 3+ TFLOP/s in DP
- 6+ TFLOP/s in SP
- Up to 16 GiB MCDRAM
- ≥ 400 GB/s MCDRAM bandwidth
- Up to 384 GiB DDR4 RAM
- ≥ 90 GB/s DDR4 bandwidth
- Supports common OS
- Register for webinar



“Standard Candle” Testbench



vs.

One Intel Xeon Phi 7120P coprocessor (2012)
TDP: 300 W, RCP: $4129

Two Intel Xeon E5-2697 v3 CPUs (2014)
TDP: 290 W, RCP: $5404

See also “Intel Xeon Product Family: Performance Brief”

§3. Computation and Optimization

Optimization Methodology

Optimization Areas

- Scalar optimization
- Vectorization
- Multi-threading
- Memory access
- Communication

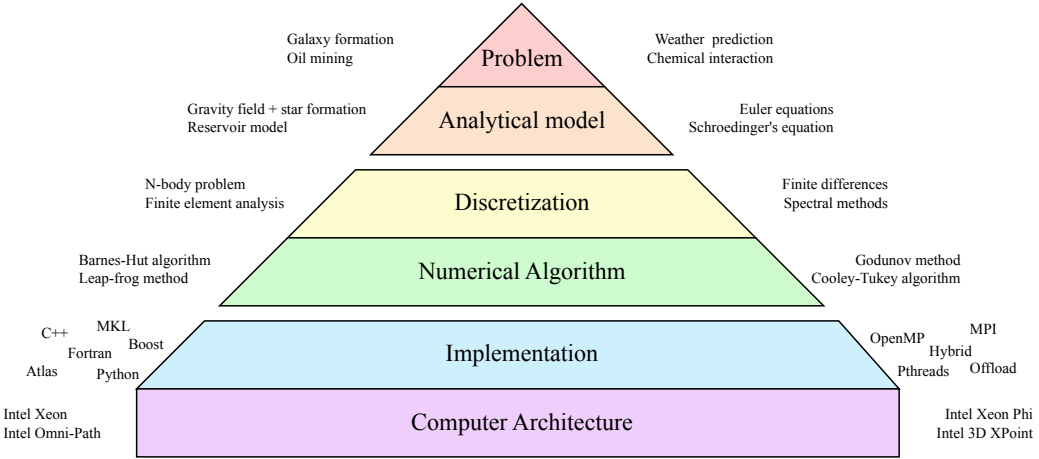
Details in HOW Series + our book.

How to Navigate Them

1. Focus on the algorithm
2. Achieve parallel scalability
3. "Hotspot-guided optimization": iteratively use VTune + optimization report

Performance and Algorithms

Computing in Science and Engineering



Algorithm Optimization Tips

1. Instead of re-inventing the wheel, call standard library functions (e.g., instead of matrix-matrix multiplication with loops, use MKL)
2. Identify bad asymptotic computational complexity (e.g., $O(N^3)$) and use improved algorithms
3. Look for parallelism in the problem, expose it in the outer loops

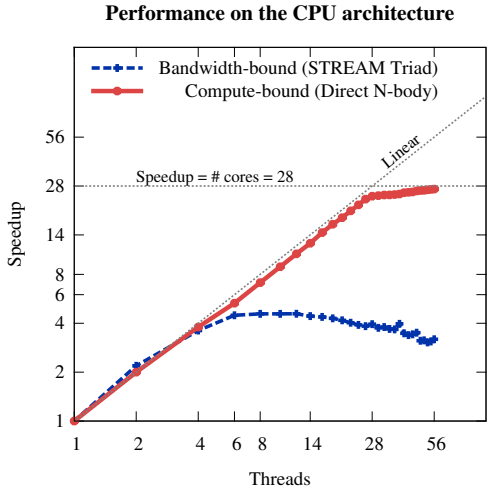
Scalability Tests

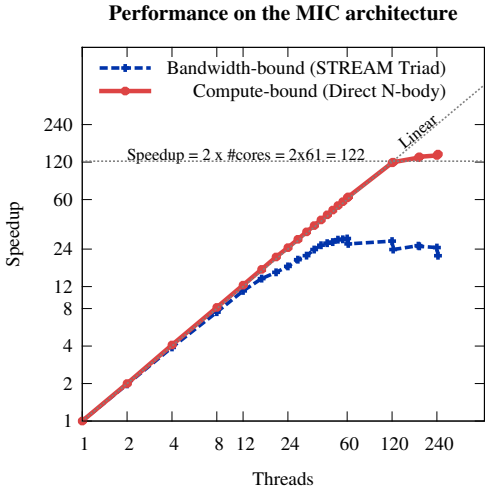
Study Thread Scalability with OpenMP

1. Set `KMP_AFFINITY=compact`
   If hyper-threading is enabled, use `compact,1` or `scatter`
2. Vary `OMP_NUM_THREADS` from 1 to # of logical CPUs
3. On Xeon Phi, use `KMP_PLACE_THREADS`

- Expectation depends on problem: compute- or bandwidth-bound
- VTune to detect location of imbalance, synchronization, overhead

Expected Thread Scalability





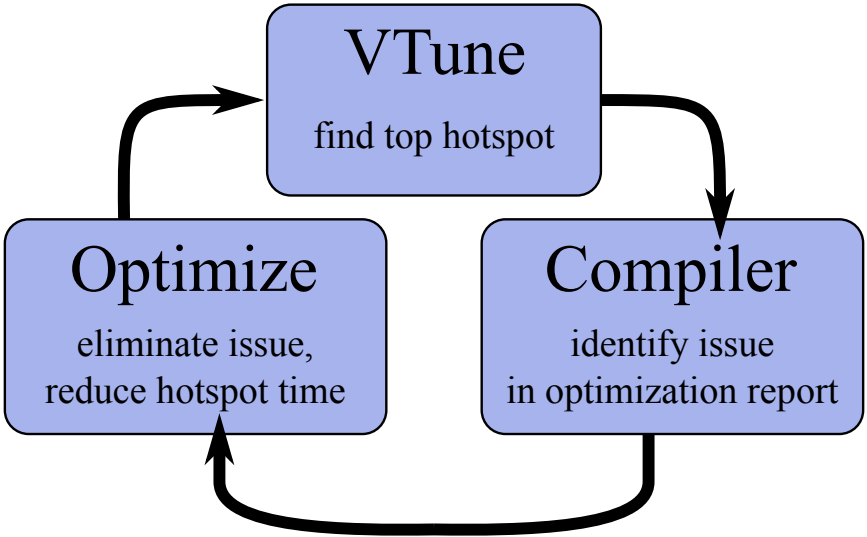
Study Vector Scalability

1. Compile code with `-no-vec -no-simd`
2. Alternatively, use `#pragma novector` in code

- Speedup equal to vector width = good
- Less than vector width = no vectorization or memory-bound
- VTune to detect most important loops for vectorization

Hotspot-Guided Optimization

Hotspot-Guided Optimization



Using Intel VTune Amplifier XE

1. Compile code with `-g -O2` or `-g -O3`
2. Set environment variables or use a wrapper script
3. Tweak code input for a short representative run

- Advanced hotspots – good starting point
- Focus on optimization report for detected hotspots

Clues in Optimization Report

1. Compile code with `-qopt-report`
2. For more verbosity, use up to `-qopt-report=5`

Things to look for:

- Failed vectorization
- Peeling in short vector loops
- Strided load/store on CPU = gather/scatter on MIC
- Type conversions
- Multiversioning in vectorized loops
- Suggestions for loop permutation

VTune to detect most important locations.

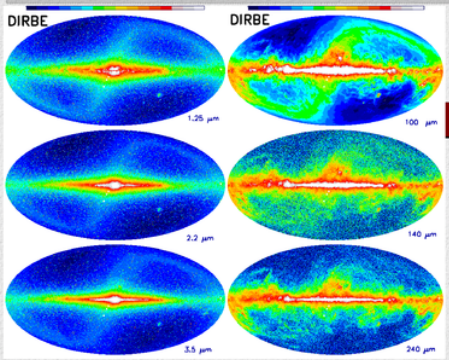
Optimization Report Example

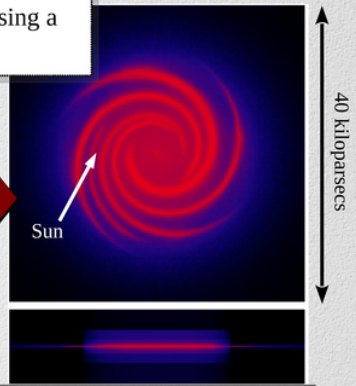
```
LOOP BEGIN at TransientHeatingFunctionsXeonPhi.cc(162,4)
   remark #15389: vectorization support: reference bMatrix has unaligned access
   remark #15389: vectorization support: reference _M_data has unaligned access
   remark #15381: vectorization support: unaligned access used inside loop body
   remark #15305: vectorization support: vector length 8
   remark #15399: vectorization support: unroll factor set to 2
   remark #15309: vectorization support: normalized vectorization overhead 1.118
   remark #15417: vectorization support: number of FP up converts: single prec..
   remark #15300: LOOP WAS VECTORIZED
   remark #15442: entire loop may be executed in remainder
   remark #15450: unmasked unaligned unit stride loads: 2
   remark #15475: --- begin vector loop cost summary ---
   remark #15476: scalar loop cost: 10
   remark #15477: vector loop cost: 2.120
   remark #15478: estimated potential speedup: 3.890
   remark #15487: type converts: 1
   remark #15488: --- end vector loop cost summary ---
LOOP END
```


§4. Case Study: HEATCODE

Case Study: Building a 3D Model of the Milky Way Galaxy using 2D Sky Surveys

Goal: build a 3D model of the Milky Way Galaxy using a large volume of 2D data from sky surveys.





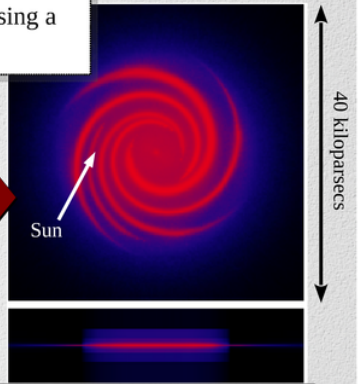
One of possible realizations of 3D models of the Milky Way Galaxy (cosmic dust luminosity map calculated by the FRaNKIE code)

Case Study: Building a 3D Model of the Milky Way Galaxy using 2D Sky Surveys

Goal: build a 3D model of the Milky Way Galaxy using a large volume of 2D data from sky surveys.

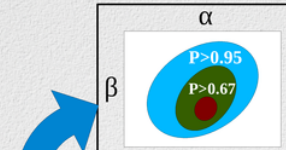
Method: Bayesian inference. Simulate the Galaxy, assess the fit to data, refine 3D model parameters, rinse & repeat.

Challenge: modeling the process of stochastic heating of cosmic dust by starlight, in each voxel of a 3D grid, is very time consuming.
With unoptimized code, **hundreds of CPU-years** for each run.

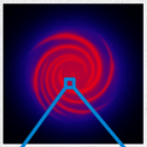


One of possible realizations of 3D models of the Milky Way Galaxy (cosmic dust luminosity map calculated by the FRaNKIE code)

Software Stack for Modeling Galactic 3D Structure



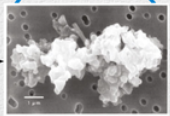
MultiNest
Bayesian analysis engine
Scales to O(10) nodes



FRaNKIE
radiation transport Monte Carlo
Scales to multiple cores in 1 node

CPU

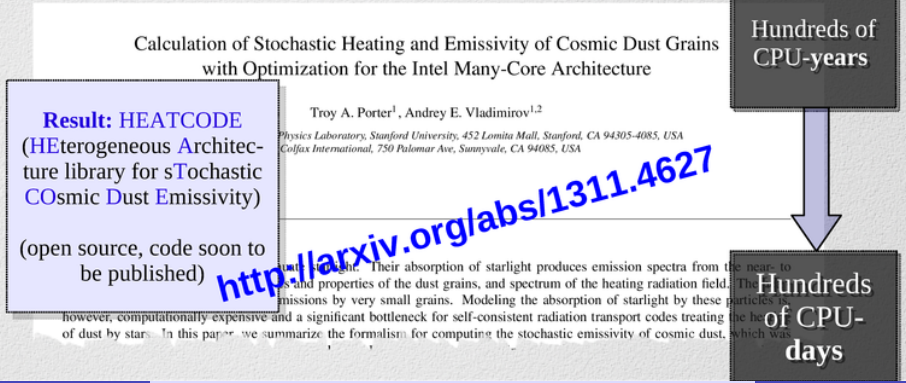
Xeon
Phi



HEATCODE
cosmic dust heating library
Multiple Xeon Phi coprocessors in 1 node

Accelerating Radiation Transport Models for the Milky Way

Solution: use a computing accelerator, optimize existing code.



Result: HEATCODE (HEterogeneous Architecture library for sTochastic COsmic Dust Emissivity)

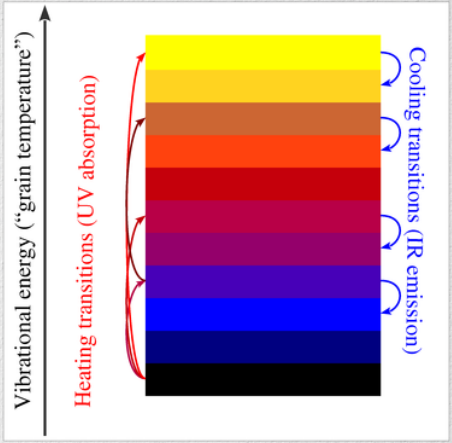
(open source, code soon to be published)

Hundreds of CPU-years

Hundreds of CPU-days

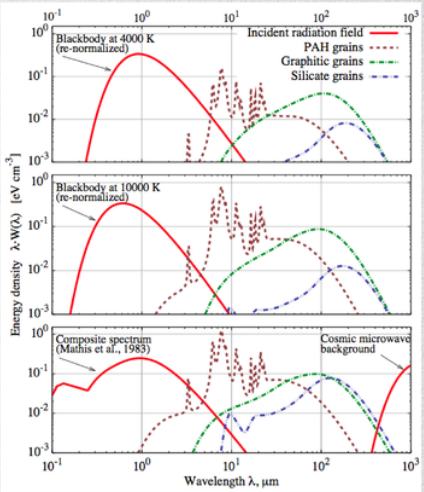
Stochastic Dust Grain Heating

- Small grains (≤0.1 μm) are important
- Absorption and re-emission is stochastic (non-thermal)
- Grains undergo "temperature" spikes, characterized by temperature distribution
- Evaluation is computationally expensive



Calculation of Stochastic Dust Emissivity

- **Input**: incident electromagnetic radiation field
- **Intermediate**: “temperature” distribution of grains of all sizes
- **Output**: spectrum of re-emitted photons
- Method and absorption cross sections: Draine et al. (2001), ApJ, 551, 807



Matrix Formalism for Stochastic Dust Emissivity

- **Stage 1:** Interpolate (in log space) and convolve the incident RF with the photon absorption cross sections

$$T_{ul} = I(\lambda)\sigma(\lambda)\frac{\lambda^3 \Delta E_{ul}}{hc^2} \quad \text{for} \quad u > l.$$

$$I(\lambda)\sigma(\lambda) \equiv \Omega(\lambda)$$

$$\log\left[\frac{\Omega(\lambda)}{\Omega(\lambda_{j-1})}\right] = \frac{\log\left(\lambda/\lambda_{j-1}\right)}{\log\left(\lambda_j/\lambda_{j-1}\right)} \log\left[\frac{\Omega(\lambda_j)}{\Omega(\lambda_{j-1})}\right]$$

transcendental operations

- **Stage 2:** form and solve a quasi-triangular system of linear algebraic equations for the "temperature" distribution

$$\sum_{j \neq i} T_{ij} P_j - \sum_{j \neq i} T_{ji} P_i = 0$$

$$T_{ij} = 0, \quad \text{if} \quad i < j - 1$$

$$B_{fj} = \sum_{k=f}^{M} T_{kj} \quad (f > j)$$

$$X_f = \frac{1}{T_{(f-1)f}} \sum_{j=0}^{f-1} B_{fj} X_j$$

sparse memory access

- **Stage 3:** convolve the "temperature" distribution with the grain size distribution and emissivity function

$$\nu F_a(\nu) = \sigma(\nu) \sum_{i=0}^{M} P_i(a) \Lambda(\nu, E_i)$$

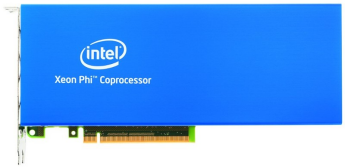
$$\Lambda(\nu, E_i) = \begin{cases} 0, & \text{if} \quad E_i < h\nu, \\ \dfrac{2h\nu^4}{c^2} \dfrac{P_i}{\exp(h\nu/kT_i) - 1} \end{cases}$$

$$\nu F(\nu) = \int_{a_{\min}}^{a_{\max}} \nu F_a(\nu) Q(a) da$$

dense linear algebra

§5. Practical Optimization

“Standard Candle” Testbench



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See also “Intel Xeon Product Family: Performance Brief”

Focust Point 1: Algorithm

- Before: 3 nested loops — $O(N^3)$ complexity
- After: 2 nested loops — $O(N^2)$ complexity
- Used recurrent relation to improve algorithm

Speedup in HEATCODE: 3.7x

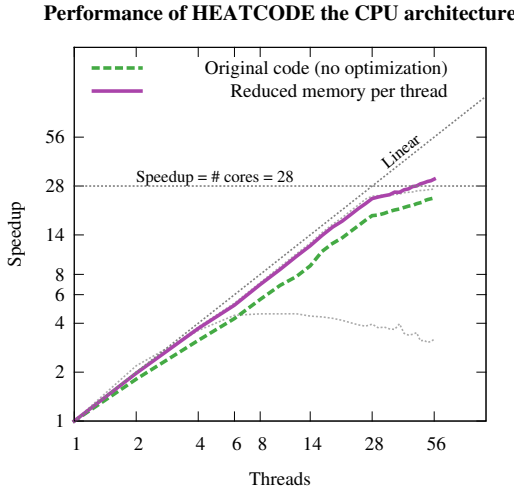
Focus Point 2: Thread Scalability

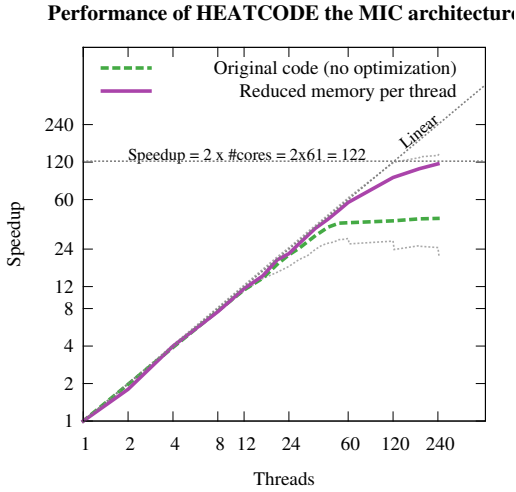
- Minimize synchronization
- Tune scheduling for load balancing
- Expose all of the parallalelism
- Make threading co-exist with vectorization

Speedup in HEATCODE: 1.2x (total: 4.4x)

More details in the HOW series Session 4 and Session 7

HEATCODE Scalability Tuning





Fruit 1: Algebraic Optimization

- **Precompute + look up** vs **Compute on time** — tradeoff
- Rule of thumb: 100 FLOPs = 1 memory access
- Precomputation helped in HEATCODE

Speedup in HEATCODE: 4.3x (total: 19x)

Fruit 2: Scalar Tuning

- All double precision = OK
- All single precision = GREAT
- Mixed precision = BAD

Speedup in HEATCODE: 1.8x (total: 34x)

More details in the HOW series Session 6.

Fruit 3: Memory Traffic

- Loop tiling: cache blocking or unroll-and-jam
- Cache-oblivious parallel recursion
- Loop fusion

Speedup in HEATCODE: 2.4x (total: 82x)

More details in the HOW series Session 9.

Fruit 4: Vectorization

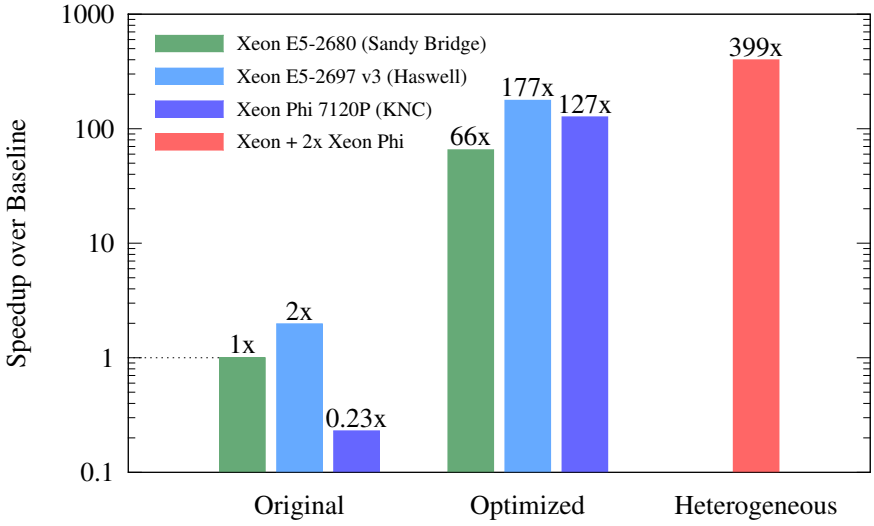
- Data alignment
- Alignment hint
- Guiding the compiler with `#pragma simd`

Speedup in HEATCODE: 1.1x (total: 91x)

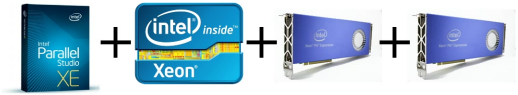
More details in the HOW series Session 6.

§6. Summary

Performance Results



Illustration



Porting to Intel® Xeon Phi™ coprocessors

- We ported Frankie code using explicit offload model
- Same code & optimization methods for Xeon Phi™
- Simultaneous calculations on CPU and coprocessors with automatic load balancing was easy to implement
- With two Intel® Xeon Phi™ coprocessors, performance for high-res calculations is 3.2x better than with two Intel® Xeon® E5 processors alone.
- RESULT: estimated target project calculation time is now 2 weeks (down from 6+ years)

Goal achieved!

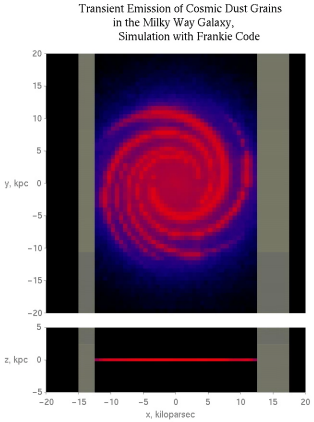


Illustration: youtu.be

Paper: http://xeonphi.com/papers/heatcode

Optimization Methodology

Optimization Areas

- Scalar optimization
- Vectorization
- Multi-threading
- Memory access
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How to Navigate Them

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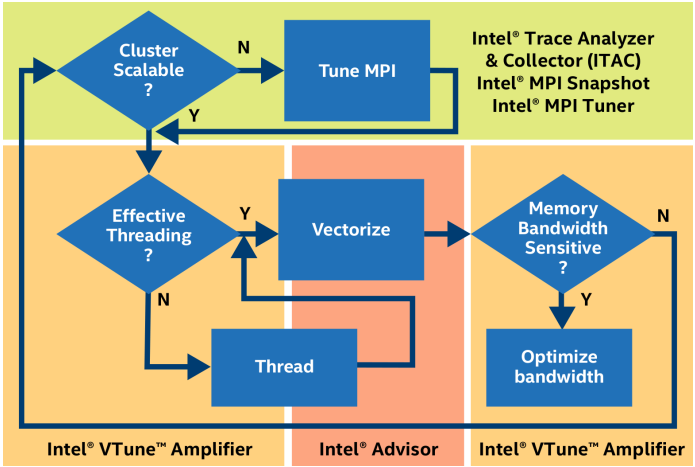
Alternative Optimization Methodology



Source: Parallel Universe Magazine, issue 23

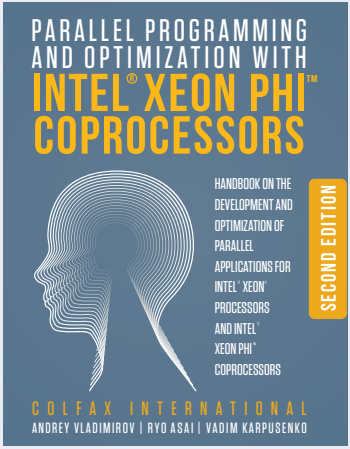
§7. Resources

Supplementary Materials: Textbook

ISBN: 978-0-9885234-0-1 (2nd edition, 508 pages, Electronic or Print)

Parallel Programming
and Optimization with
Intel® Xeon Phi™
Coprocessors

Handbook on the Development and
Optimization of Parallel Applications
for Intel® Xeon® Processors
and Intel® Xeon Phi™ Coprocessors



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