Challenges for Developing & Supporting HPC Applications

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Its More than Programming

- HPC Applications are about solving problems
- Programming is only one small(ish) part that includes
  - Data management (input, output, visualization, analytics, …)
  - Performance and correctness debugging
  - Integration with workflows
  - And yes, dealing with limitations in programming systems and their implementations, particularly the growing diversity in architectures

Speakers

- Torsten Hoefler, ETH Zürich
  - Automatic compiler-driven GPU acceleration with Polly-ACC
- Jeffrey Hollingsworth, University of Maryland
  - Bugs and Speed in HPC Applications: Past, Present, and Future
- Michela Taufer, University of Tennessee, Knoxville
  - Modeling the Next-Generation High Performance Schedulers

HPC Application Lifecycle (Partial)

- Design
  - Choice of mathematical models
  - Choice of algorithms
- Implementation
  - Choice of programming approaches
  - Choice of Libraries and the use of code analysis tools
- Testing
  - Correctness
  - Performance (and do you know what the achievable performance is?)
- Science workflow
  - Creating input data and analyzing output data - includes mesh generation (e.g., CFD) or data partitioning (e.g., bioinformatics)
  - Run ensembles for uncertainty quantification, parameter sweeps, nonlinear optimization, …
- Repeat each step in all combinations…

Real Challenges in Programming

- For HPC, we are looking for high performance
  - FLOPS and Memory Bandwidth ("roofline" https://dl.acm.org/citation.cfm?id=1498785)
  - FLOPS and Memory Bandwidth and Latency (Execution-Cache-Memory (ECM) model https://link.springer.com/chapter/10.1007%2F978-3-642-14390-8_64)
  - FLOPS and Memory Bandwidth and Instruction Rate ("Achieving high sustained performance in an unstructured mesh CFD application" https://dl.acm.org/citation.cfm?id=331600 , 1999)
- Node performance is often key (in 1999 result above – 7x performance improvement from memory locality on the node)
- In distributed memory programming, the challenge is managing the distributed data structures and the operations upon them
  - It would be great if a programming language provided ***your*** data structure (and some are close) but the reality is that most apps have specific needs

Managing Code Transformations

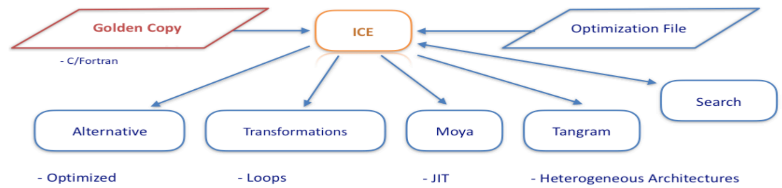
- Many tools exist (some you'll hear about today)
- Need a way to
  - Separate additional abstractions (e.g., loop count is small) vs. proscriptive requirements (e.g., unroll loop by 3)
  - Invoke multiple tools
    - Transformation generators, autotuners, …
  - Remember good (and bad!) choices of parameters, transformations, etc. by system/input/characterization
  - Provide ways to confirm transformations preserve correctness

What is Correctness?

- How do we know that the performance portable code is correct?
  - Or even if it will compute the same result as the original code
    - And what is “the same result”?
- It is *not enough* to prove that any code transformations are correct
  - MPICH used to test whether the compiler returned the same result in a and c for these two statements:
    - ```
      a = joe->array[OFF+b+1];
      c = joe->array[OFF+1+b];
      ```
  - Because one major vendor compiler got this ***wrong***.
- And you still need to prove that the hardware implements all of the operations correctly
  - And vectorization is already likely to produce results that are not bitwise identical to the non-vector version (which might depend on how data is aligned at runtime)
- Question: How do you test that the performance portable code is computing what is intended?
- Proving code transformations correct is *necessary* but not *sufficient*
      ```

Illinois Coding Environment (ICE)

- One pragmatic approach
- Assumptions
  - Fast code requires some expert intervention
  - Can't all be done at compile time
  - Original code (in standard language) is maintained as reference (***Golden Copy***)
  - Can add information about computation to code
- Center for Exascale Simulation of Plasma-Coupled Combustion
  - http://xpacc.illinois.edu



- Approach
  - Annotations provide additional descriptive information
    - Block name, expected loop sizes, etc.
  - Source-to-source transformations used to create code for compiler
    - Exploit tool ecosystem – interface to existing tools
    - Original "Golden Copy" used for development, correctness checks
  - Database used to manage platform-specific versions; detect changes that invalidate transformed versions

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Stencil 3D

```
#pragma @ICE loop=stencil
for(i = 1; i < x-1; i++) {
  for(j = 1; j < y-1; j++) {
    for(k = 1; k < z-1; k++) {
      B[i][j][k] = C0 * A[i][j][k] + C1 * (
                   A[i+1][j][k] + A[i-1][j][k] +
                   A[i][j+1][k] + A[i][j-1][k] +
                   A[i][j][k+1] + A[i][j][k-1]);
    }
  }
}
#pragma @ICE endloop
```

+

```
---
#Built command before compilation
prebuildcmd:

#Compilation command before tests
buildcmd:
    make realclean;  make CC={compiler} COPT={params}

buildoptions:
   gcc:
        params:{'-O':{'default': 3,'min': 0,'max': 3}}
   icc:
        params:{'-O':{'default': 3,'min': 0,'max': 3}}

#Command call for each test
runcmd: ./sten3d 1024 20

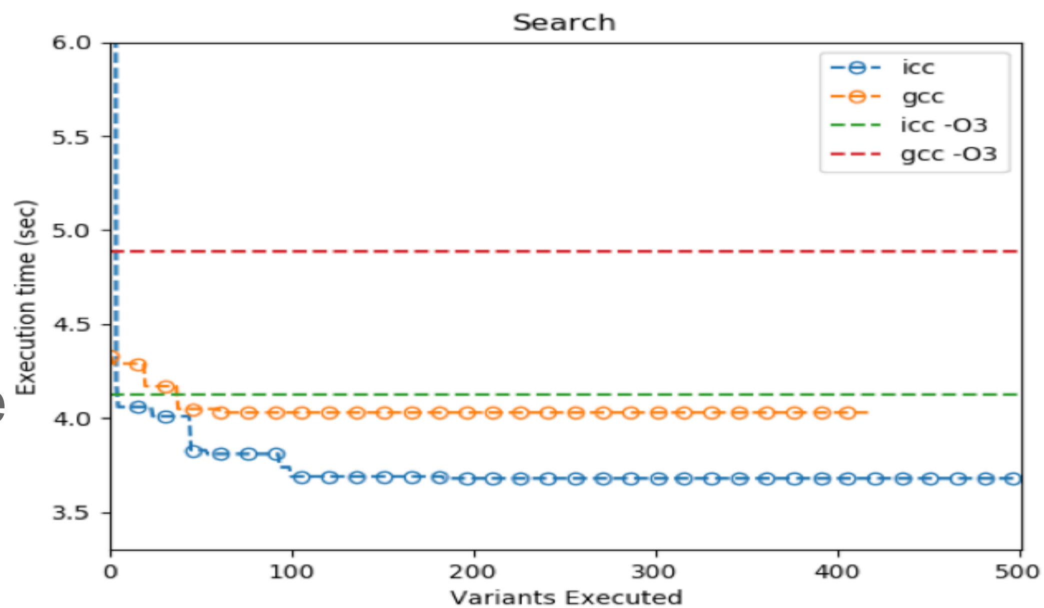
tuning: on

stencil:
       rose_uiuc:
          - stripmine+:
              loop: 4
              factor: 16..1024
                type: poweroftwo
          - stripmine+:
              loop: 3
              factor: 16..1024
                type: poweroftwo
          - stripmine+:
              loop: 2
              factor: 16..1024
                type: poweroftwo
          - interchange+:
              order:0,1,3,5,2,4,6
...
```

Work of Thiago Teixeira and David Padua

Performance Results

- 3-D Stencil
  - 11,664 variants
  - Max 12.6 sec
  - Min 3.68 sec
  - Speedup over simple code
    - icc: 1.12x
    - gcc: 1.21x



Summary

- HPC Applications require many kinds of support over their lifetime, *especially* beyond programming
- Many tools and approaches exist
  - A challenge is to make these tools work together
- (though I have not discussed this) HPC and “Big Data” environments share problems and solutions
  - MPI and scalable algorithms for collective operations from HPC used in ML
  - Data systems and tools from big data offer better capabilities and user productivity for HPC
  - Only a start here. Both sides have much to learn and to offer