The Intel Parallel Computing Center at the University of Bristol

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Bristol's rich heritage in HPC

The University of Bristol is one of the top HPC institutes in the UK:

- It has a vibrant HPC community of >500 researchers, >10% of all staff
- Invests over £2.5m p.a. in local HPC
- Trains over 100 HPC computer scientists each year (Bristol CS ranked #4 in UK)
HPC resources in Bristol

• Blue Crystal supercomputer:
  • £12m invested since 2006
  • Amongst the fastest in the UK
  • ~10,000 processor cores
  • ~250 TFLOPS
  • >1 PetaByte of data storage
• Bristol is a leader in the use of many-core accelerators:
  • Intel Xeon Phi
  • Nvidia, AMD GPUs
Intel chose to invest in the University of Bristol to establish its first "Intel Parallel Computing Center (IPCC)" in the UK (Feb 2014):

“The University of Bristol combines both a demonstrated ability to innovate and optimize parallel applications using open, industry-standard techniques with a focus on practical education of the next generation of application developers,”

- Joe Curley, Intel
Bristol IPCC activities

Optimising various HPC codes for Xeon Phi:

- **BUDE**
  - Molecular docking code
- **ROTORSIM**
  - Multi-block, multi-grid CFD code
- **CloverLeaf/TeaLeaf**
  - Hydrodynamics benchmark
- **Lattice Boltzmann and more**
BUDE (Bristol University Docking Engine) is one of the fastest and most accurate molecular docking codes in the world.

BUDE is being used to find new drug targets for influenza, malaria, Alzheimer's, Emphysema, Insulin signalling and more.

"High Performance in silico Virtual Drug Screening on Many-Core Processors", S. McIntosh-Smith, J. Price, R.B. Sessions, A.A. Ibarra, IJHPCA 2014
BUDE's algorithm

1: function DOCK(protein, ligand)
2:   Generate initial population poses at random
3:   energies = COMPUTE_ENERGIES(protein, ligand, poses)
4:   for each iteration of EMC do
5:     Select poses with lowest energies as parents
6:     Generate new population poses from parents
7:     energies = COMPUTE_ENERGIES(protein, ligand, poses)
8:   end for
9:   Output best poses
10: end function

11:

12: function COMPUTE_ENERGIES(protein, ligand, poses)
13:   for i = 0 upto size(poses) - 1 do
14:     Transform ligand by poses[i]
15:     energies[i] = 0
16:     for each atom l_atom in ligand do
17:       for each atom p_atom in protein do
18:         energies[i] = energies[i] + INTERACTION(p_atom, l_atom)
19:       end for
20:     end for
21:   end for
22:   return energies
23: end function
BUDE's conditional behaviour

\[ E_{\text{complex}} = E_{\text{steric}} + E_{\text{electrostatic}} + E_{\text{desolvation}} + E_{\text{config\_entropy}} \]
if (a > b)
{
    accumulator += (a - b*c);
}

setp.gt.f32 %pred, %a, %b
@!%pred bra $endif
mul.f32 %f0, %b, %c
sub.f32 %f1, %a, %f0
add.f32 %accumulator, %accumulator, %f1
$endif:

temp = (a - b*c);
mask = (a > b ? 1 : 0)
accumulator += (mask * temp);

mul.f32 %f0, %b, %c
sub.f32 %temp, %a, %f0
setp.gt.f32 %pred, %a, %b
selp.f32 %mask, %one, %zero, %pred
mad.f32 %accumulator, %mask, %temp, %accumulator
More BUDE optimisations for Phi

- Work-group and NDrange sizes are very important (multiples of 16, 240 etc.)
- Lots of input into Xeon Phi OpenCL driver
  - Have seen a 2-3X improvement in last year
- Vtune on Phi proving very useful
BUDE Xeon Phi results

One Xeon Phi SE10P **1.94X** faster than 16 cores of Sandy Bridge at 3.1GHz
Cloverleaf: A Lagrangian- Eulerian hydrodynamics benchmark

• A bandwidth-limited structured grid code that is part of Sandia's "Mantevo" benchmark suite
• Solves the compressible Euler equations, which describe the conservation of energy, mass and momentum in a system.
• These equations are solved on a Cartesian grid in 2D with second-order accuracy, using an explicit finite-volume method.
• Optimised parallel versions exist in OpenMP, MPI, OpenCL, OpenACC, CUDA and Co-Array Fortran
CloverLeaf optimisations for Xeon Phi

• Focused on OpenCL and OpenMP
• Task granularity is crucial
  • Important to get rid of bounds checking
• Memory alignment and access patterns are also very significant
  • Many simultaneous memory streams can cause the TLBs to thrash
• Barrier placements critical
  • Adding barriers can improve performance
Vtune can be really useful on Phi
CloverLeaf Xeon Phi results

Summary

• Bristol is a leader in exploiting many-core architectures to deliver cutting-edge HPC

• Xeon Phi can deliver acceleration of 1.5-2.0X for real HPC codes

• There's a very worrying trend that many HPC codes are not evolving fast enough to be ready for the many-core trend
  
  • Implication: these codes will fail to get good performance on Xeon, never mind Xeon Phi!
OpenCL conference in Bristol

http://iwoocl.org

- IWOCL ("eye-wok-ul")
- May 12-13\textsuperscript{th} 2014
- Bristol, UK
- In an award-winning science museum
- 2 days of technical talks and workshops