

Geilo Winter School 2008

Henrik Löf Uppsala Universitet



Optimizing parallel applications

- Low latencies (locality of reference)
 - Cache memories
 - -Remote Accesses (NUMA)
- Low parallel overhead
 - -Minimize communication and synchronization
- Load Balance
 - Partitioning
 - -Each thread has an equal amount of work



Uniform Memory Access (UMA)



- Server
 - Few dozen CPU/cores
 - Easy to administrate
- Volume product
- Uniform access time
 - "Easy" to understand
- •Examples
 - SMP
 - CMP
- Scalability problems
 - Limited interconnect bandwidth



- Physically Distributed Memory
 - Shared memory programming
- Cluster of UMA nodes
 - CPU boards
 - Multi socket CMP systems
- Better scalability
 - Maintaines simpler shared memory programming model
- Examples
 - Sun Fire 15K, 25K
 - SGI Origin/Altix
 - HyperTransport (AMD)
 - QuickPath (Intel)
- Expensive



CPU



Sun WildFire, a Distributed Shared Memory (DSM) System





Sun WildFire what it looks like







Local access – fast!





UNIVERSITET

Local access – fast!





Remote access – slower!





Remote access – slower!





NUMA-ratio



 $NUMA - ratio = \frac{T_{remote}}{T_{remote}}$ local



Implementing Conjugate Gradients in OpenMP



Analyzing CG

Given an initial guess x_0 , store $r_0 = b - Ax_0$ and set $p_0 = r_0$. do k = 0,1,K(1) Store Ap_{k} (2) Store $\langle p_k, Ap_k \rangle$ (3) $\alpha_k = \frac{\langle r_k, r_k \rangle}{\langle p_k, Ap_k \rangle}$ $(4) \quad x_{k+1} = x_k + \alpha_k p_k$ $(5) \quad r_{k+1} = r_k - \alpha_k A p_k$ (6) Store $\langle r_{k+1}, r_{k+1} \rangle$ (7) $\beta_k = \frac{\langle r_{k+1}, r_{k+1} \rangle}{\langle r_k, r_k \rangle}$ (8) $p_{k+1} = r_{k+1} + \beta_k p_k$









UNIVERSITET

Basic parallelization of CG



Basic parallelization of CG

cg_iter_count = 1

do

call SpMxV(A,p,temp)

pAp_norm = 0.0_rfp

do i = 1, matrix_size
 pAp_norm = pAp_norm + p(i)*temp(i)
end do

alpha = r_old_norm/pAp_norm

x(:) = x(:) + alpha * p(:) r_new(:) = r_old(:) - alpha * temp(:)

.



UPPSALA UNIVERSITET

Basic parallelization of CG

!\$OMP PARALLEL DEFAULT(SHARED) PRIVATE(cg_iter_count)

cg_iter_count = 1

do

call SpMxV(A,p,temp)

```
!$OMP SINGLE
    pAp_norm = 0.0_rfp
!$OMP END SINGLE
!$OMP DO REDUCTION(+:pAp_norm)
    do i = 1, matrix_size
        pAp_norm = pAp_norm + p(i)*temp(i)
        end do
!$OMP END DO
```

```
!$OMP SINGLE
alpha = r_old_norm/pAp_norm
!$OMP END SINGLE
!$OMP WORKSHARE
x(:) = x(:) + alpha * p(:)
r_new(:) = r_old(:) - alpha * temp(:)
!$OMP END WORKSHARE NOWAIT
```



Sun EIOK

€

CPU

400MHz US-II + UMA

DRAM

€

CPL





Serial









Serial 220s

Sun EI0K







Serial 220s

Serial

Sun EI0K



























Geographical Locality

- Property of an application
 - -"How many memory accesses are node-local?"
 - Communication
- Dependent on many things
 - -Data distribution (source code/OS)
 - -Thread scheduling (OS)
- Thread-data affinity: Minimize the amount of remote accesses by co-location of threads and data



Problems of initialization

- FEM assembly process serial
- First-touch strategy
 - -All data allocated on a single node
- Access pattern stored in the data
 - -Compressed Sparse Row (CSR)
 - Efficient parallel initialization not possible
- We need ways of redistributing data during runtime


Code modifications

- Inserted affinity-on-next-touch call before the first CG iteration
- Access pattern is static cross the iterations
 - -Only need to redistribute once
- Used hardware counters to quantify effect



16 threads



16 threads



16 threads



Analysis, affinity-on-next-touch

- Proper data distribution important
 - -Every iteration 2.61 times faster
- Overhead
 - -Cold start effects
 - -Cost of migration



- Overhead is amortized over iterations
- Scalability better, still poor
 - -Speedup 9 on 28 threads



Overall effect of affinity-on-nexttouch



Number of Threads





affinity-on-next-touch + 64Kb



affinity-on-next-touch + 64Kb 3s







Algorithmic Optimizations (CG)

- Bandwidth minimization
 - -Increases cache utilization
- Load Balance
 - -Graph partitioning (MeTiS)
- Removing barriers
 - -Reduces parallel overhead
- How do they interact with data distributions?



Removing Barriers

- Standard implementation uses 7 barriers
- 4 barriers can be removed
 - Privatizing scalars
 - -Reording initializations of reduction variables
 - -3 global barriers in total
- S-step methods (Chronopoulos/Gear)
 - Introduces another vector to calculate two iterations simultaneously
 - -Only one reduction necessary
 - -2 global barriers in total
 - -No numerical problems



Bandwidth Minimization

- Graph theoretical method
 - -Reverse Cuthill-McKee
 - -Gibbs-Poole-Stockmayer (GPS)
- Permutes matrix to minimize bandwidth
- Small bandwidth increases locality
 - -Larger part of RHS cache blocks utilized





Bandwidth Minimization

- Graph theoretical method
 - -Reverse Cuthill-McKee
 - -Gibbs-Poole-Stockmayer (GPS)
- Permutes matrix to minimize bandwidth
- Small bandwidth increases locality
 - -Larger part of RHS cache blocks utilized





Load Balance, example





UNIVERSITET

2

3

Load Balance, example





Load Balance and Partitioning

- In OpenMP partitions are linear
 - A chunk of rows (indeces) is associated with a thread
 - -No care is taken to the number of non-zeros
- Graph partitioning partitions the non-zeros more evenly
 - -Used in message-passing applications
- Results:
 - -Graph partitioning increased matrix bandwidth which led to poor locality
 - Bandwidth minimization toghether with standard OpenMP produced very good partitions



Load balance of SpMxV



16 partitions	Base	GPS	MeTiS
Max(non_zeros)/Avg(non_zeros)	1.24	1.01	1.15



16 partitions	Base	GPS	MeTiS
Max(non_zeros)/Avg(non_zeros)	1.24	1.01	1.15



Load balance of SpMxV



Number of non-zeros per row

16 partitions	Base	GPS	MeTiS
Max(non_zeros)/Avg(non_zeros)	1.24	1.01	1.15



Uniform system, EI0K



Number of Threads



Non-uniform system (SFI5K) with data distribution



Number of Threads



Conclusions, algorithmical optimizations

- Locality most important
 - -Bandwidth minimization
- Bandwidth minimization also produced load balanced partitions
- Graph partitioning increased the amount of remote accesses
- Load balance and synchronization overheads are of secondary importance



- Many applications exhibit dynamic and/or unstructured access patterns
 - -Commercial Software
 - -Adaptive Mesh Refinement (AMR)
- For these applications, clever initializations will not be optimal
 - –We need some kind of migration/replication mechanism



UPPSALA UNIVERSITET

Model problem

- $\frac{\partial u}{\partial t} = a \frac{\partial u}{\partial x} + b \frac{\partial u}{\partial y}$
- Periodic boundaries
- Finite differences
 - -2^{nd} order in space
 - 4th order R-K in time
- Blockwise AMR
- Written in Fortran 90/95
- Parallelized using OpenMP





AMR movie





Solver Algorithm

```
do t=1,Nt
  if (t mod adaptInterval=0) then
       Estimate error per block.
       Adapt blocks with inappropriate resolution.
       Repartition the grid.
      Migrate blocks (if migration is activated).
  end if
  F1=Diff(u);
  F2=Diff(u+k/2*F1)
  F3=Diff(u+k/2*F2)
  F4=Diff(u+k*F3)
  u=u+k/6*F1+k/3*F2+k/3*F3+k/6*F4
end do
```



- The blocks needs to be assigned to threads in a way that balance the work (partitioning)
 - Domain based partitioning won't do the job since the pulse moves across the domain
 - -We used the Jostle diffusion partitioner
- Our problem:
 - We need to make sure that the data in each partition is physically allocated on the node where the corresponding thread executes



- Four nodes
 - Four CPUs per node
- Bound threads
 - I.UMA
 - 2. NUMA
 - 3. NUMA-MIG
- The amount of remote accesses quantifed using CPU hardware counters











- Four nodes
 - Four CPUs per node
- Bound threads
 - I.UMA
 - 2. NUMA
 - 3. NUMA-MIG
- The amount of remote accesses quantifed using CPU hardware counters









- Four nodes
 - Four CPUs per node
- Bound threads
 - I.UMA
 - 2. NUMA
 - 3. NUMA-MIG
- The amount of remote accesses quantifed using CPU hardware counters











- Four nodes
 - Four CPUs per node
- Bound threads
 - I.UMA
 - 2. NUMA
 - 3. NUMA-MIG
- The amount of remote accesses quantifed using CPU hardware counters











- Four nodes
 - Four CPUs per node
- Bound threads
 - I.UMA
 - 2. NUMA
 - 3. NUMA-MIG
- The amount of remote accesses quantifed using CPU hardware counters





Results

	UMA	NUMA	NUMA-MIG
Total time	4.09 h	6.64 h	3.99 h
L2 miss rate	4.3%	3.9%	4.2%
Remote accesses	0.2%	62.9%	8.1%

- Geographical locality has a significant effect!
- Dynamic page migration works!



Execution Time

Effect of data migration




Streamline Simulation









Segments

1

39





















	4	5	
	3		
1	2		











		6	7	
	4	5		
	3			
1	2			





Streamline Storage

- The geometry of the streamlines is stored as a sequence of coordinates
- To store the streamlines we have several options
- I. Allocate huge array and hope for the best
- 2. Use a dynamic array or a linked list
- 3. Trace once to count the segments, allocate an array and trace again













Segments Regularized Grid



















Segments





































Streamlines and Shared Memory

- To extract parallelism we trace, solve and map for several streamlines concurrently
 - -You can extract fine-grained parallelism from a single streamline
- We call a set of streamlines a streamline bundle or simply bundle
- We seek a parallel algorithm that minimizes parallel overhead
 - -Communication
 - -Load imbalance
 - -Synchronization





Parallel Algorithm

Algorithm 1 Parallel Streamline Simulation

Require: $T_{end} \leftarrow \text{simulation end time}$

Require: $dt \leftarrow$ global timestep

Require: $T \leftarrow dt$

- 1: repeat
- 2: Solve pressure equation
- 3: Calculate velocity field
- 4: repeat
- 5: Select launch points for streamlines and build bundle
- 6: Assign launch points in bundle to threads
- 7: **for all** streamlines in bundle **do**
- 8: 1:st trace, count segments
- 9: 2:nd trace, pick up pressure grid data, store the segments
- 10: Build streamline grids from segment and pressure grid data
- 11: Solve the corresponding 1-D transport equations
- 12: **end for**
- 13: Map new values of the transport variables to the pressure grid
- 14: **until** Domain is sufficiently covered
- 15: $T \leftarrow T + dt$

16: **until** $T \ge T_{end}$





Thread 1 Thread 2


















































Static Assignment





Thread 1 Thread 2













































































Thread 1 Thread 2





Thread 1 Thread 2



We have to enforce mutual exclusion

We ha



Thread 1 Thread 2



We have to enforce mutual exclusion



Hamster

- Single-phase tracer flow
- Uniformly refined CCAR grid
- Streamlines are implemented in a way comparable to most industrial codes (3DSL, FrontSim)
 - SPU upwinding scheme for I-D solves
 - Simple averaging scheme for mapping
 - Dual trace for storing segments
 - 2-point flux approximation (7-point stencil)
 - GMRES solver preconditioned using BoomerAMG from the HYPRE package
 - Tracing using Pollock's method



Test Case #1, SPE10

- We cut out a domain of size 32x128x32 from the bottom 32 layers of SPE10
 - 131,072 cells
- One global time step of 2000 days (~5 years)
- I0,096 streamlines

- Production well at constant BHP of 4000 psi
- Injection well at constant BHP of 10000 psi





Streamline Statistics, SPEI0

	Min	Max	Median	Average	Std.Dev
Number of Segments	77	203	103	107	106
Number of Iterations	Ι	6296	19	119	244





Performance on 4 way dual-core Opteron

Threads	Execution Time (s)	Speedup
1	12.01	1.00
2	6.64	1.82
4	3.74	3.23
8	2.21	5.70



Scalability Problems

- Did not take NUMA into account
 - Linux does not yet support page migration
- Cell and face ordering on unstructured grids
 - -Every cache line should be used
 - -Communication
 - -False sharing





Performance on Sun Niagara 2 (UltraSPARC-T2)

Threads	Execution Time (s)	Speedup
1	84.40	1.00
2	42.44	1.99
4	21.36	3.95
8	10.91	7.73
16	6.27	13.47
32	3.81	22.15
64	157.88	0.53



Manual (Optimal) Load Balancing

- In the static case, we can improve load balance by assigning a weight representing the compute time
- We then formulate a discrete optimization problem using these weights
- Possible parameters for load balancing weights
 - I. Rock properties (segment counts)
 - 2. Total time of flight (iterations)
 - 3. Well placement (segment count)
 - 4. Size of multi-phase region (flash calculations)
 - 5. Cache misses and communication costs (hardware)



Load Balanced Algorithm

Algorithm 2 Load Balanced Streamline Simulation
Require: $T_{end} \leftarrow$ simulation end time
Require: $dt \leftarrow \text{global timestep}$
Require: $T \leftarrow dt$
1: repeat
2: Solve pressure equation
3: Calculate velocity field
4: repeat
5: Select launch points for streamlines and build bundle
6: Assign launch points in bundle to threads
7: for all streamlines in bundle do
8: 1:st trace, count segments
9: 2:nd trace, pick up pressure grid data, store the segments
10: end for
11: Load balance bundle
12: for all streamlines in bundle do
13: Build streamline grids from segment and pressure grid data
14: Solve the corresponding 1-D transport equations
15: end for
16: Map new values of the transport variables to the pressure grid
17: until Domain is sufficiently covered
18: $T \leftarrow T + dt$
19: until $T \ge T_{end}$



Tracing



Tracing





Tracing



No Load Balancing





Tracing



No Load Balancing



Load Balancing









Percentage of all streamlines moved

	8 Threads	16 Threads
SPEIO	28.9%	40.9%
ANOTHER CASE	15.6%	31.0%



Origins of non-zero structure

- Every row in the matrix corresponds to a set of cells, a small **sub-domain**
- The non-zero pattern can be controlled by reordering of the unknowns (cells)
 - Graph partitioning, Space Filling Curves, Reverse Cuthill-Mckee, ..
- Load balance can be achieved if we replace the simple N/num_threads scheme
 - Assumes an efficient a-priori load estimator
 - Area and connectivity of the sub-domains control the amount of communication needed







Domains and Streamlines

- Consider a partitioning of the pressure grid into three partitions
 - This is needed for extracting parallelism from the pressure solver
 - -Each sub-domain corresponds to set of cells or equivalently, a set of rows of the iteration matrix




Naive "Parallel" Solution

- Collect the entire velocity field of the sub-domains to a master node
- Trace all the streamlines on the master node
- Copy the streamline grids back to the other nodes – Scheduling and load balancing
- Do local transport solve
- Map back





The entire velocity field must fit in the memory of the master node

-No chance for giga-cell models

- A node generates lots of communication and the communication will be localized in time (bursty)
 – Very bad for slow interconnects
- A node can only map back streamline data to the subdomain that it owns
 - More communication needed to pass all the streamlines around in the mapping step
- Probably not very scalable



A Pipelined Solution

- For simplicity assume that we trace from left to right
- The segments of an individual streamline may cross all three domains
 - Sub-domains 2 and 3 must wait until the set of streamlines crossing sub-domain 1 have reached the boundary
 - While domains 2 and 3 trace the continuation of this set we can start tracing a new set in sub-domain 1
- In this way we can overlap or **pipeline** the tracing of the streamlines





Pipelined Algorithm

- For each processor (sub-domain), repeat:
 - I. Wait for start points
 - 2. Trace all local streamlines
 - 3. Hand-off exit points to neighbor
- Think of the sub-domains as grid cells in a coarse grid.
- Every sub-domain contains one segment
 - Which consist of smaller segments based on the actual grid cells



