Optimization of LESlie3D for the Cray X1 Architecture

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- We compare execution speeds and profiles of the CFD code LESlie3D ….
  - …. On the X1, optimized code vs. original.
  - …. On the X1 vs. on the IBM POWER4.

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The ERDC X1: “Diamond”

- 64 Cray X1 MSPs (256 SSPs)
- 60 MSPs available for computation (240 SSPs)
- 16 nodes of 4 MSPs each
- Liquid cooled
- 4.5 TB scratch space

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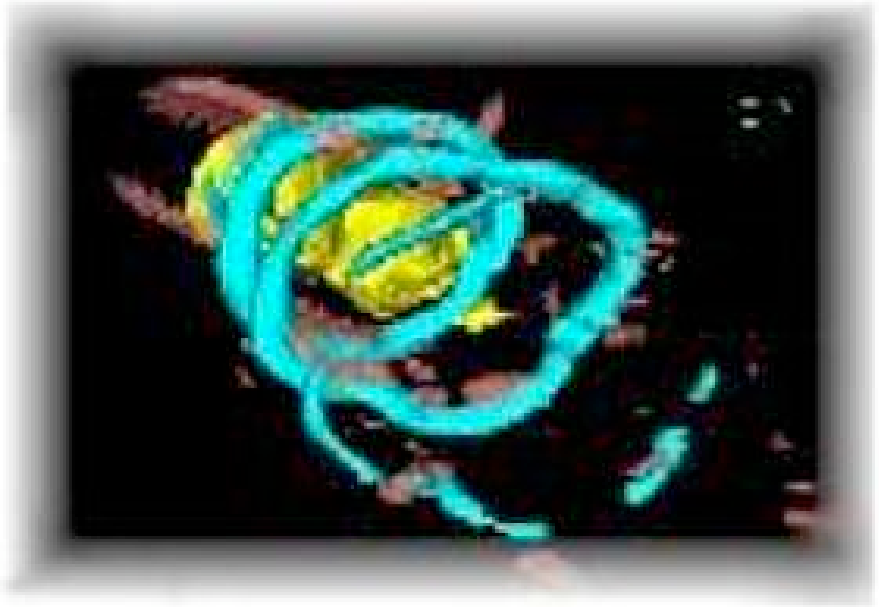
The Code: LESlie3D

Large Eddy Simulation Linear Eddy Model in 3D

- 3D Navier-Stokes solver for turbulent reacting flows (e.g. combustion), developed by Ga. Tech's Computational Combustion Laboratory
- Finite-volume predictor-corrector conservative scheme
- 4th order accurate in space; 2nd order in time
- Direct simulation mode and Large Eddy Simulation modes available



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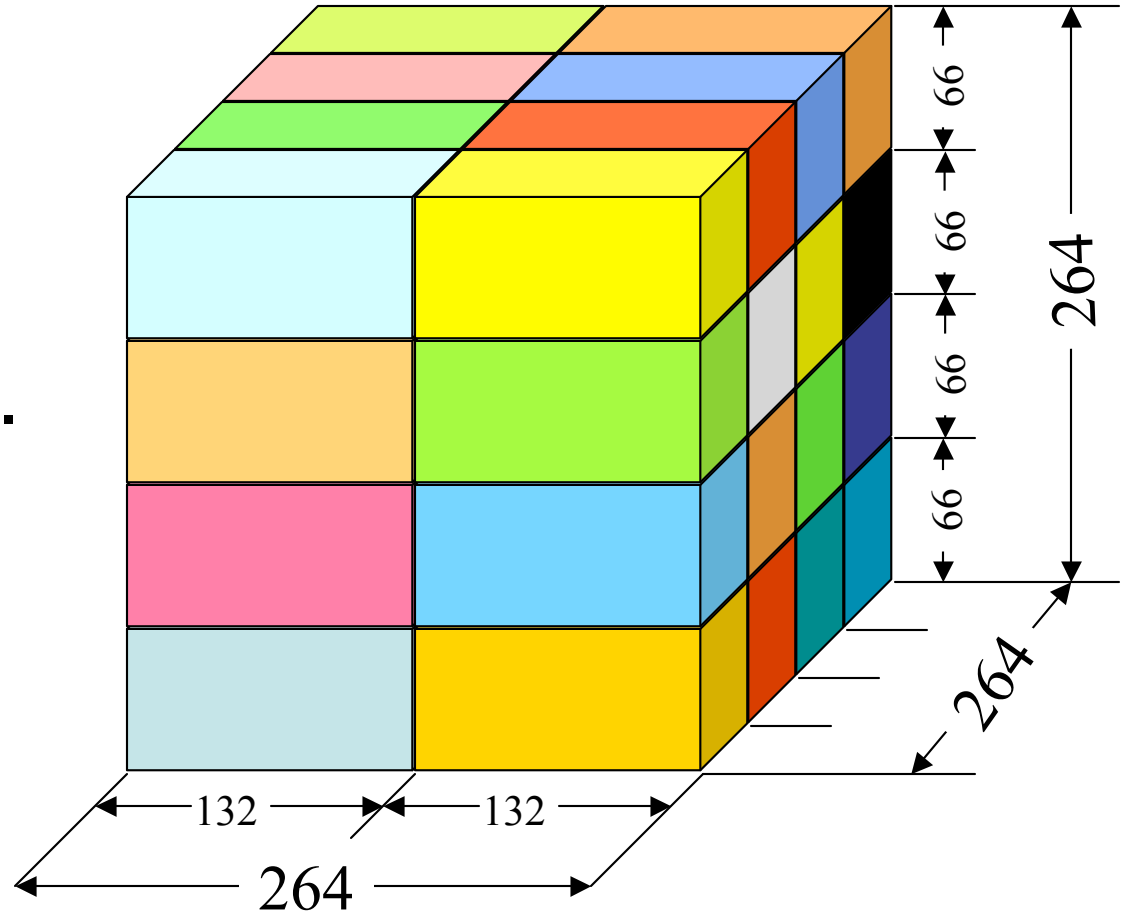
LESlie3D Divides Its Structured Mesh Into Several Structured Sub-meshes.

EXAMPLE:

264^3 mesh

With 2x4x4 PEs.



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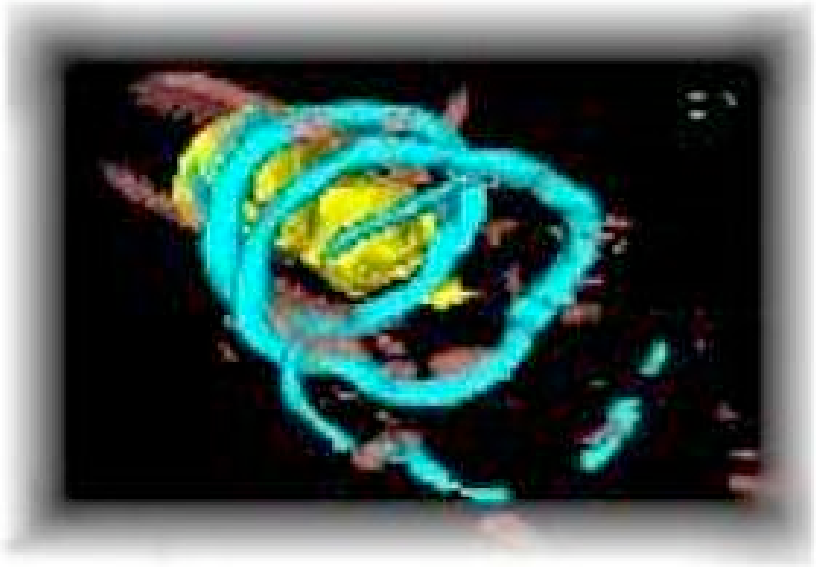
LESlie3D is a vector code, which makes it a good candidate for porting to the X1.



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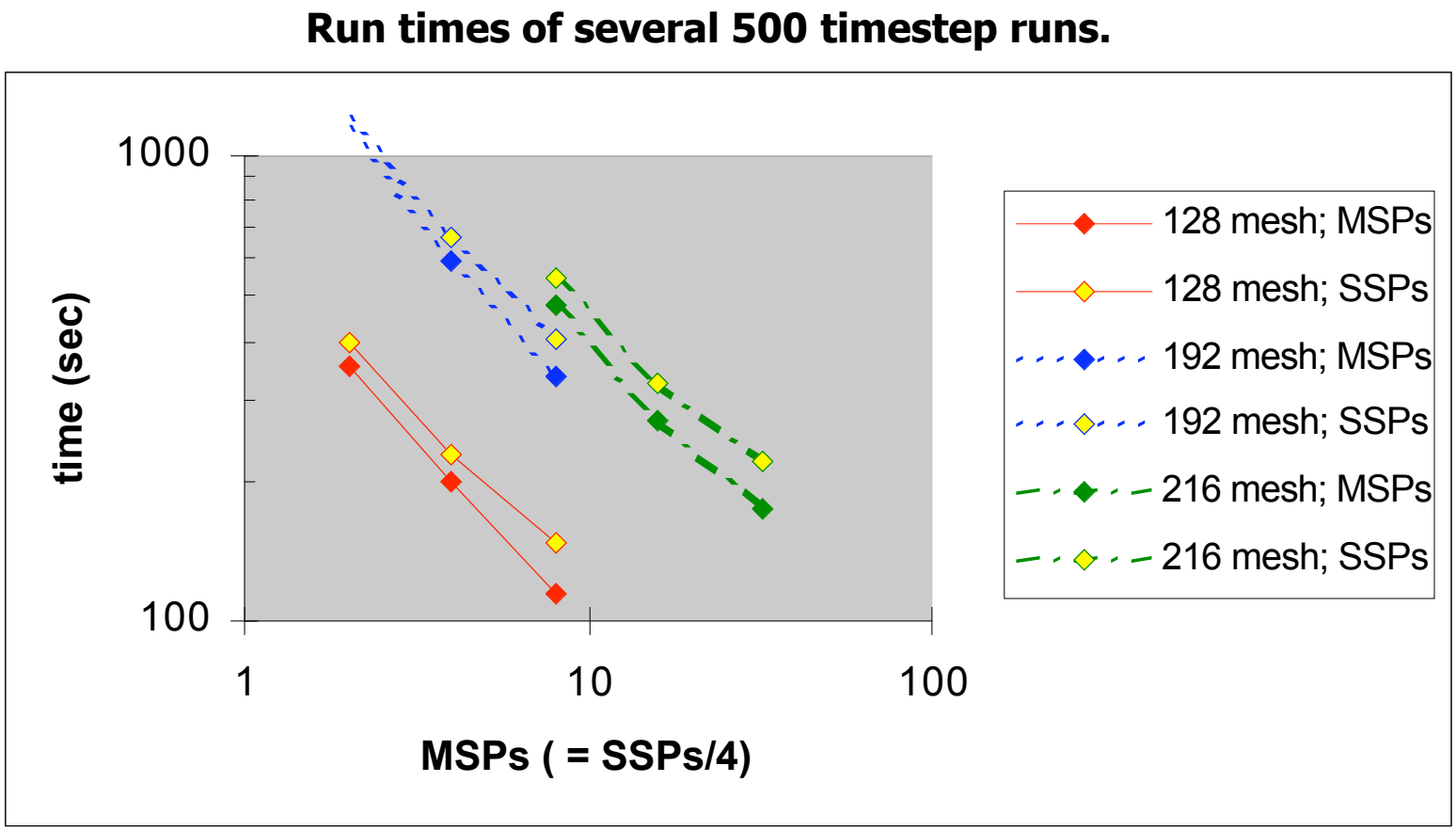
LESlie3D consistently runs faster in MSP mode than in SSP mode.



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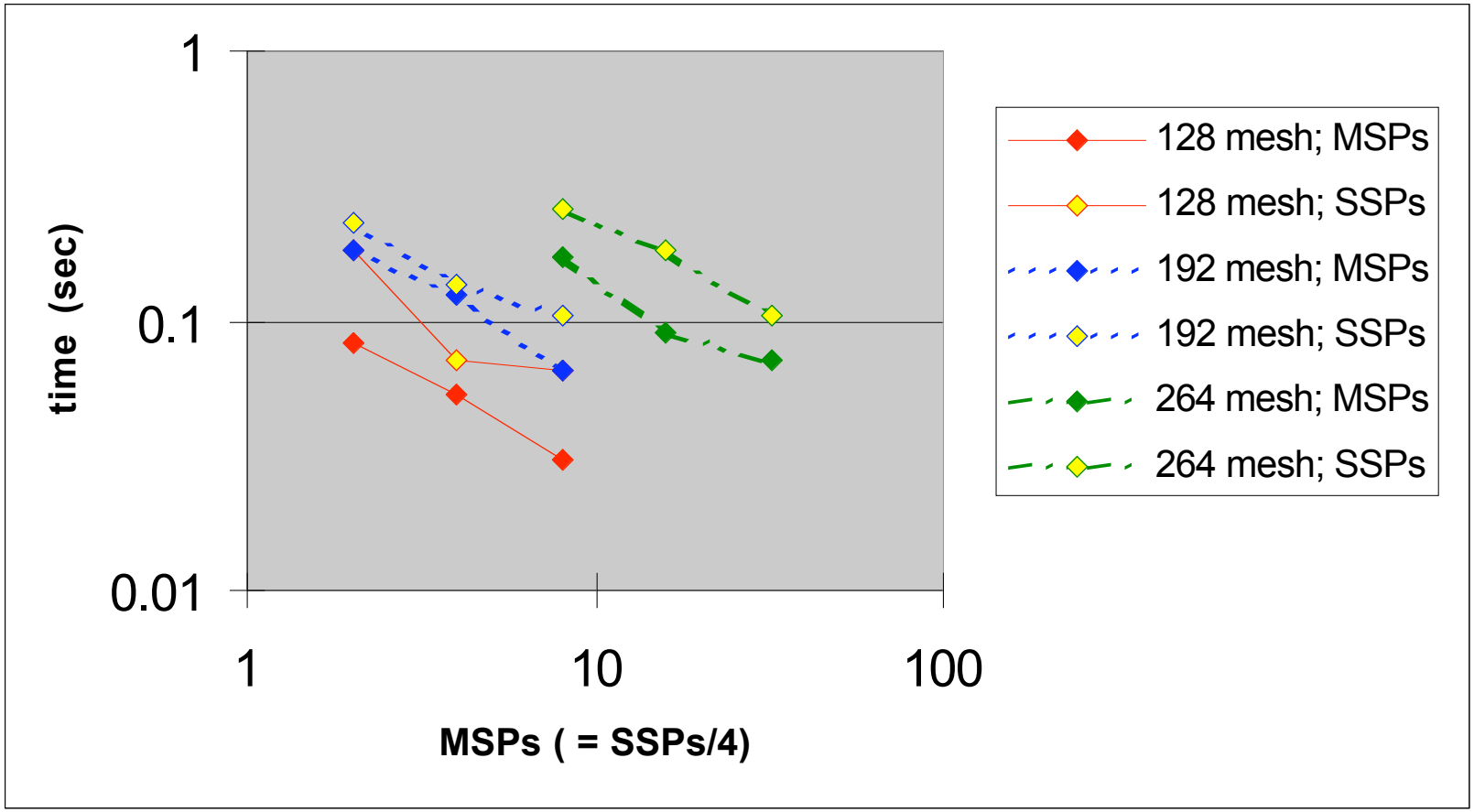
MSP mode spends less time in communication.

Communication time per timestep.



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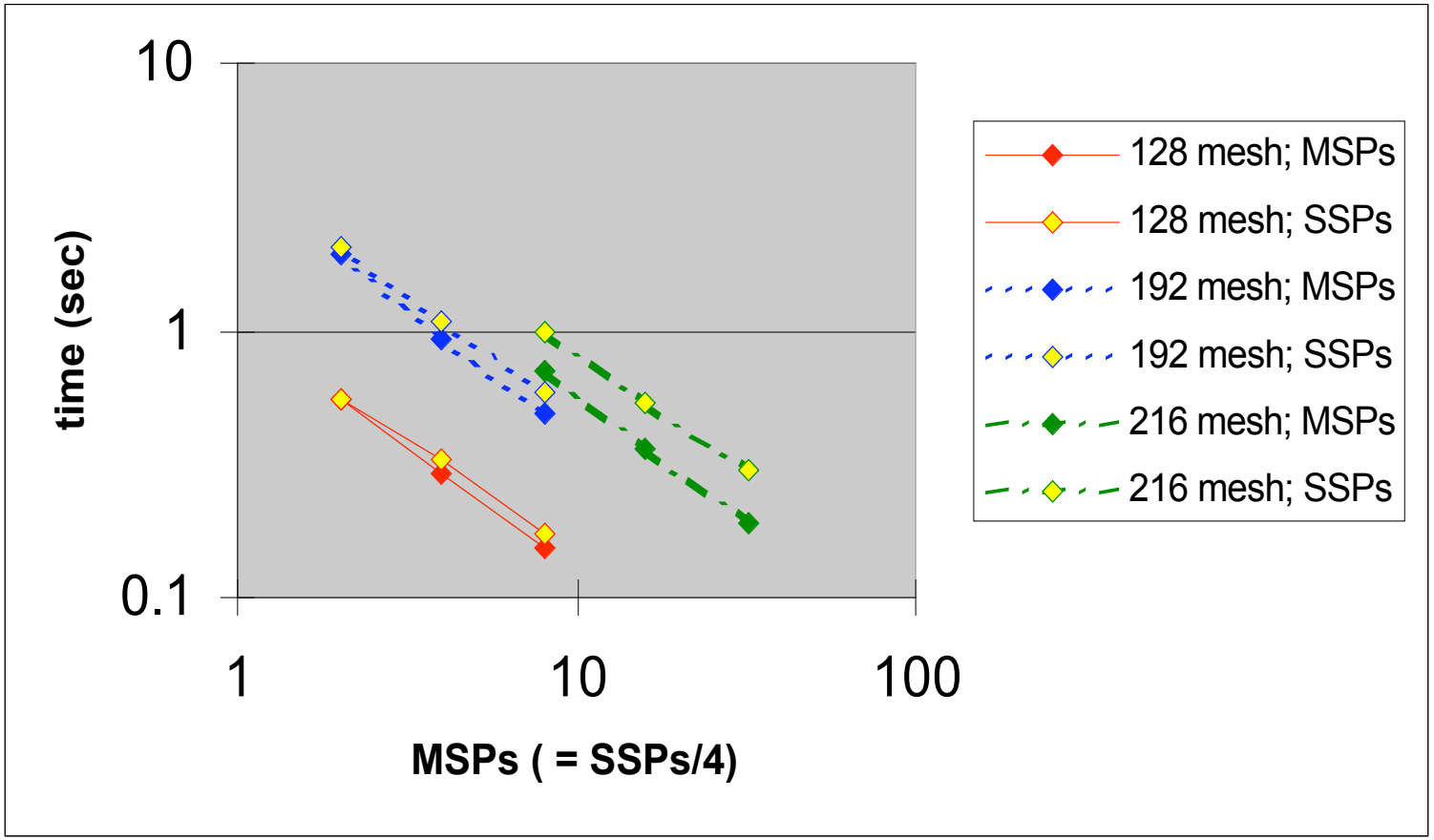
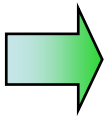
MSP runs are also faster in calculation time.

Calculation time per timestep.



Cray analysts added streaming directives to several loops to obtain multistreaming.

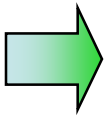
```
do k = k1,k2
  do j = j1,j2
    do i = i1,i2
           (work)
    end do
  end do
end do
```



```
!CSD$ PARALLEL DO
                PRIVATE(vars)
do k = k1,k2
  do j = j1,j2
    do i = i1,i2
           (work)
    end do
  end do
end do
!CSD END PARALLEL DO
```

Cray analysts broke up other loops to promote load balancing.

```
do nn = 1,nspeci
do k = k1,k2
  do j = j1,j2
    do i = i1,i2
         (work)
    end do
  end do
end do
end do
```



```
!CSD$ PARALLEL DO
                PRIVATE( vars )
   do kth=1,4
      k1new=k1+(k2-k1+4)/
                      4*(kth-1)
     k2new=k1new+(k2-k1+4)/
                         4 - 1
    do nn = 1,nspeci
       do k = k1new,k2new
         do j = j1,j2
           do i = i1,i2
          (work)
           end do
         end do
       end do
      (other nested loops)
     end do
  !CSD$ END PARALLEL DO
```

Cray CSD optimizations sped up LESlie3D by about 20 per cent.

	Run time		% speedup	% time in computation		% time in communication		% time in stats	
	Original	Optimized		Original	Optimized	Original	Optimized	Original	Optimized
192^3 mesh; 16 MSPs; 500 timesteps	3:29	2:47	20.10%	84.46%	78.95%	11.06%	15.42%	4.47%	5.63%
264^3 mesh; 32 MSPs; 4000 timesteps	0:44:35	0:35:56	19.40%	83.78%	76.26%	12.44%	18.99%	3.78%	4.75%

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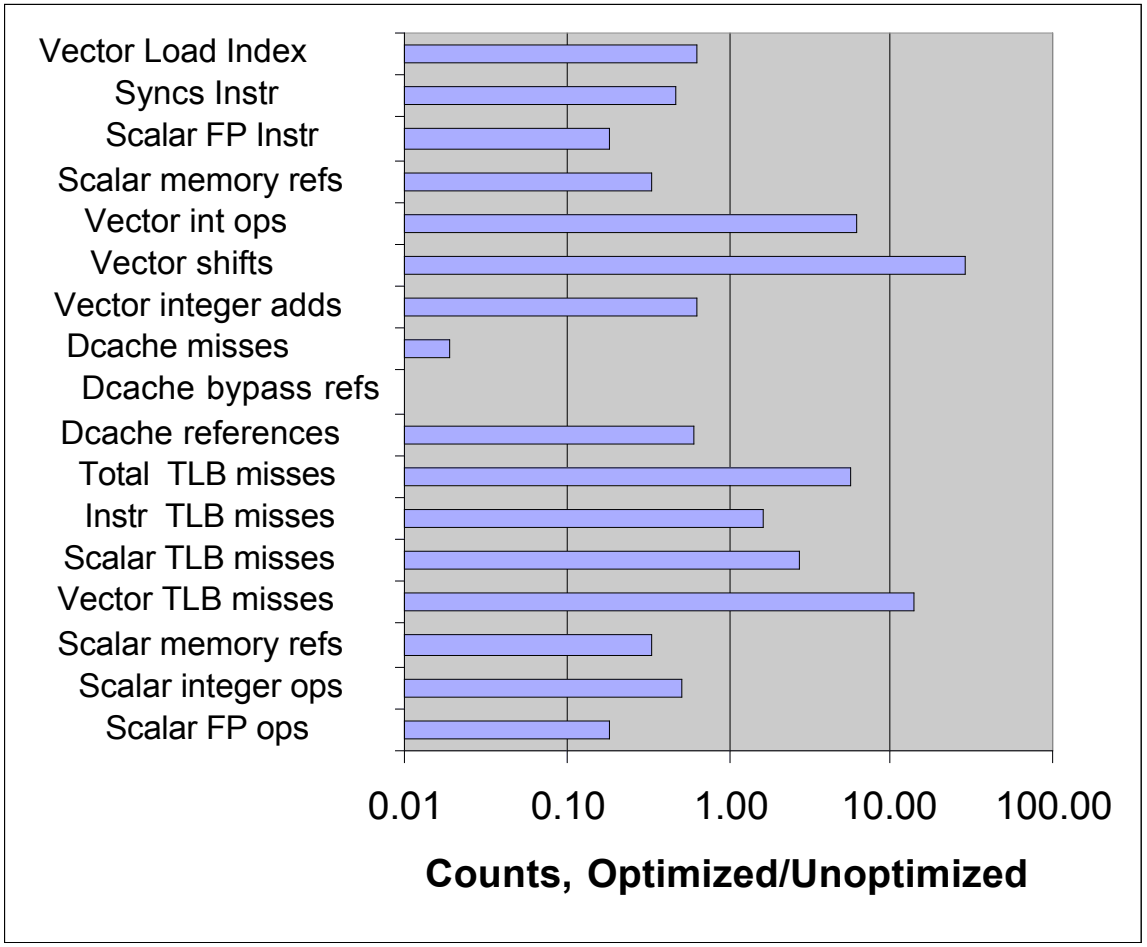
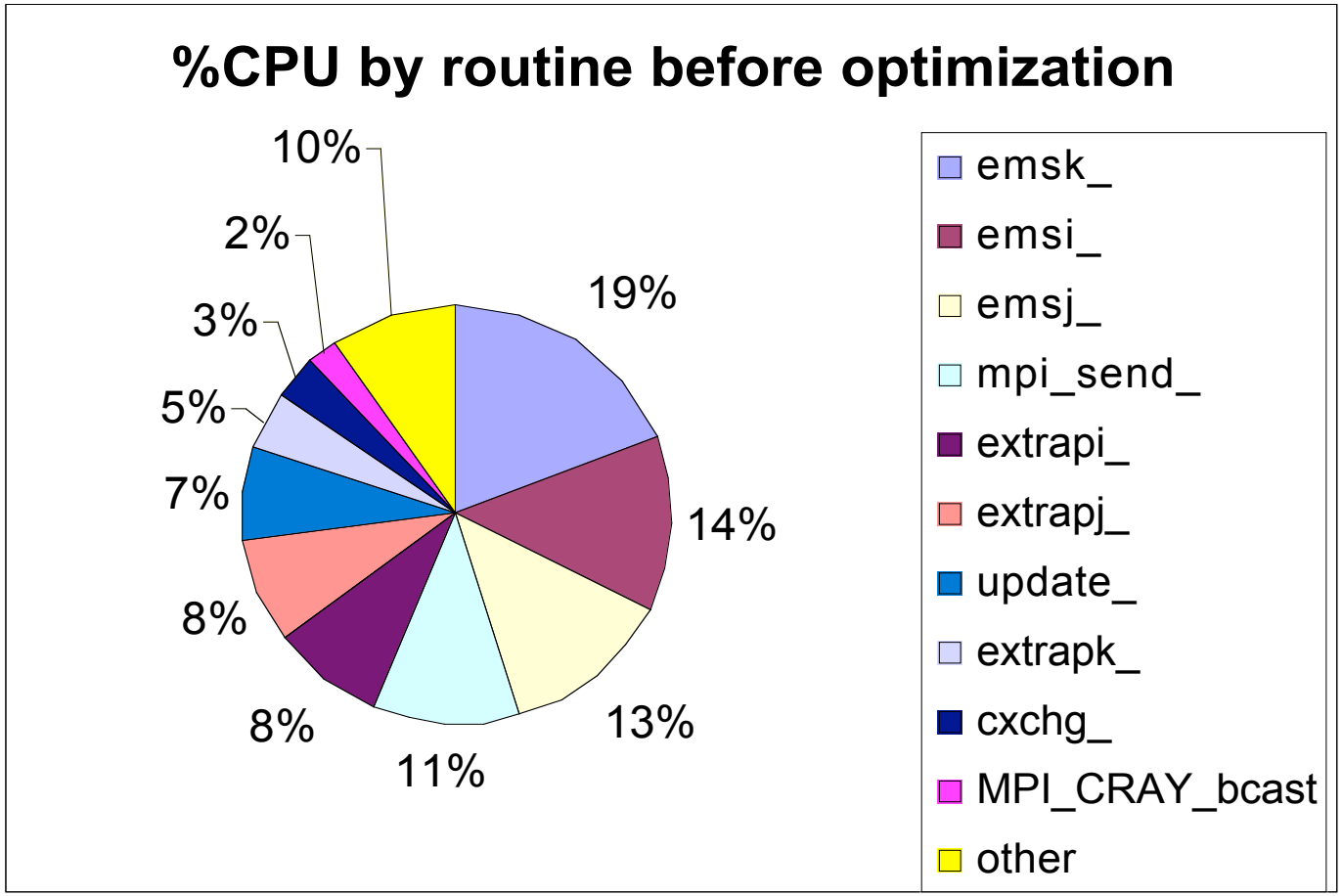
Optimization generally increased vector operations and decreased scalars.

From runs on 192^3 mesh, 1x4x4 PEs



Optimization created significant changes in performance of individual routines.



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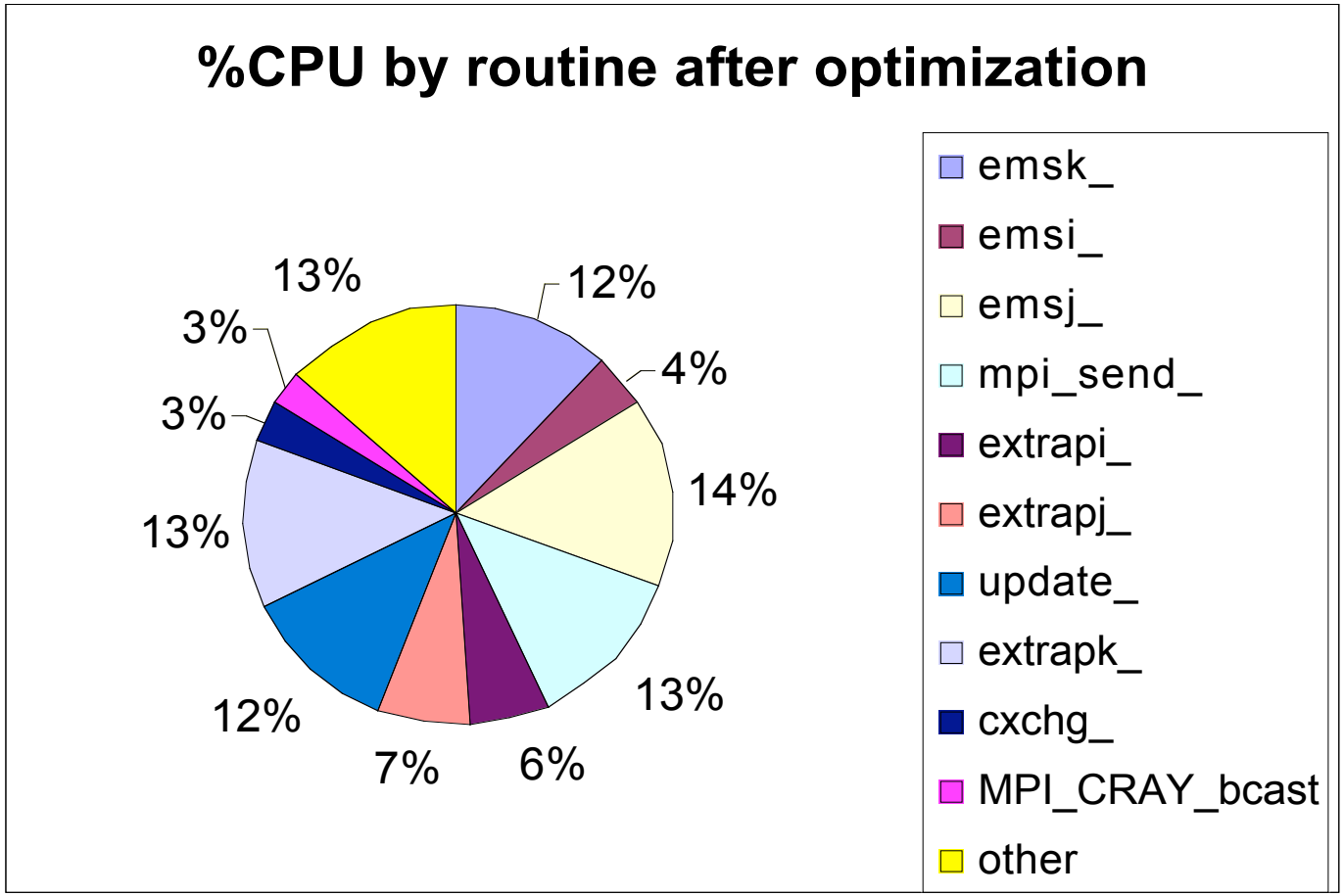

We ran LESlie3D on the X1 and the IBM P4 and compared timings.

From 192^3 mesh; 16 PEs; 500 timesteps

	X1	X1 * 4	% of total	P4	% of total
Run time (sec)	2:47	11:08		36:34	
Time per timestep	0.334	1.336	100%	4.392	100%
Calc. time per timestep	0.264	1.056	79%	3.430	78%
Comm. time per timestep	0.052	0.208	16%	0.471	11%
Stat. time per timestep	0.019	0.076	6%	0.490	11%

We have also collected hardware performance data on the Cray X1 and the IBM P4.

- X1:
- pat_hwpc counters
  - Cycles
  - Instructions graduated
  - Vector Instructions
  - Scalar memory refs
  - Vector FP adds

- P4:
- PAPI counters
  - PM_CYC
  - PM_BR_ISSUED
  - PM_FPU_ALL
  - PM_FXU_ALL
  - PM_LD_REF_L1
  - PM_FPU_FMA

Comparison is not so straightforward….

… but we did our best.

From 192^3 mesh; 16 PEs; 500 timesteps

X1 pat_hwpc counter	counts/MSP	P4 PAPI counter	counts/PE
Cycles	2.800E+11	PM_CYC	2.831E+12
Branches & Jumps	1.384E+09	PM_BR_ISSUED	1.052E+11
Branches mispredicted	3.554E+07	PM_BR_MPED_CR+ PM_BR_MPRED_TA	2.178E+09
Total FP ops	3.524E+11	PM_FPU_ALL	1.705E+11
Vector int ops + Scalar int ops	1.117E+09	PM_FXU_FIN	3.335E+11
Dcache refs	8.715E+08	PM_LD_REF_L1	3.398E+11

Conclusion

- Optimized vs. original code
  - Optimized code ran 20% faster than original.
  - Optimizations resulted in more vector operations.
- X1 vs. P4
  - The X1 outperforms the P4 by a factor of 12 at MSP level, factor of 3 at SSP level.
  - The X1 gets better hardware performance in several areas:
    - Integer ops
    - Cache
    - Branches