Parallel Software Engineering with OpenMP

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Outline

- Introduction
- What is Parallel Software Engineering
- Parallel Software Engineering Issues
- OpenMP
- KAP/Pro for OpenMP
- Conclusions

Why Parallel Software Engineering

We seek the following benefits --

- Performance
- Productivity
- Quality
- Standards

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What is Parallel Software Engineering

- Steps in Parallelizing an Application

–**A**nalyze	Find the Parallel loop. Make sure it's the right one.
–**R**e**S**tructure	Make the necessary modifications: Classify variables, Add synchronization.
–**T**est	Verify that the program basically works in parallel mode.
–**I**mprove	Do the tuning necessary to get peak performance.
–**Q/A**	Verify that the parallel application is as robust as serial application.

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Digression -- A Bit of History

- Minisupercomputers legacy
  - Sequent, Alliant pioneered in 2nd half of 80's
- PCF/X3H5 standardization effort
  - Cray, Digital, IBM, SGI developed consensus
- Parallel model used by many companies
- Advances in Shared Memory Multiprocessors is causing growing usage

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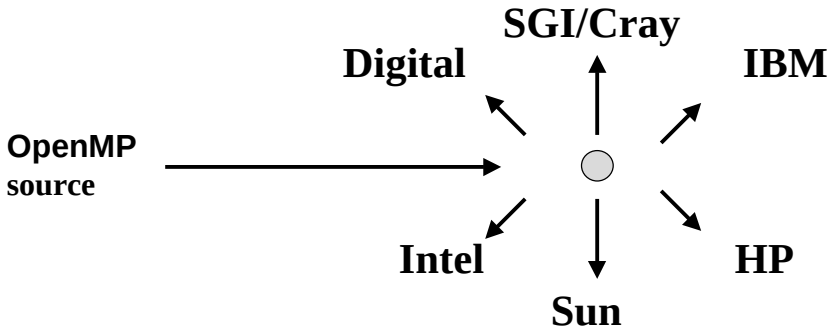
The Trend Towards *Portable* Parallel Processing

- Portability between systems.
- With a common set of directives, **OpenMP**



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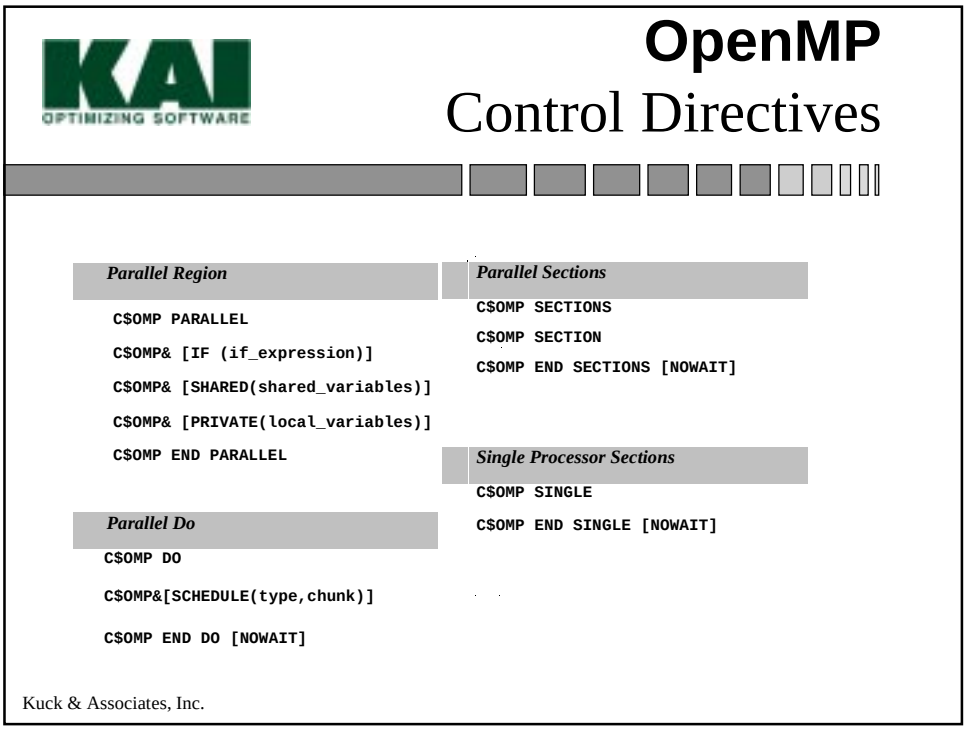
OpenMP
Control Directives
Parallel Region
C$OMP PARALLEL
C$OMP& [IF (if_expression)]
C$OMP& [SHARED(shared_variables)]
C$OMP& [PRIVATE(local_variables)]
C$OMP END PARALLEL
Parallel Do
C$OMP DO
C$OMP&[SCHEDULE(type,chunk)]
C$OMP END DO [NOWAIT]
Parallel Sections
C$OMP SECTIONS
C$OMP SECTION
C$OMP END SECTIONS [NOWAIT]
Single Processor Sections
C$OMP SINGLE
C$OMP END SINGLE [NOWAIT]
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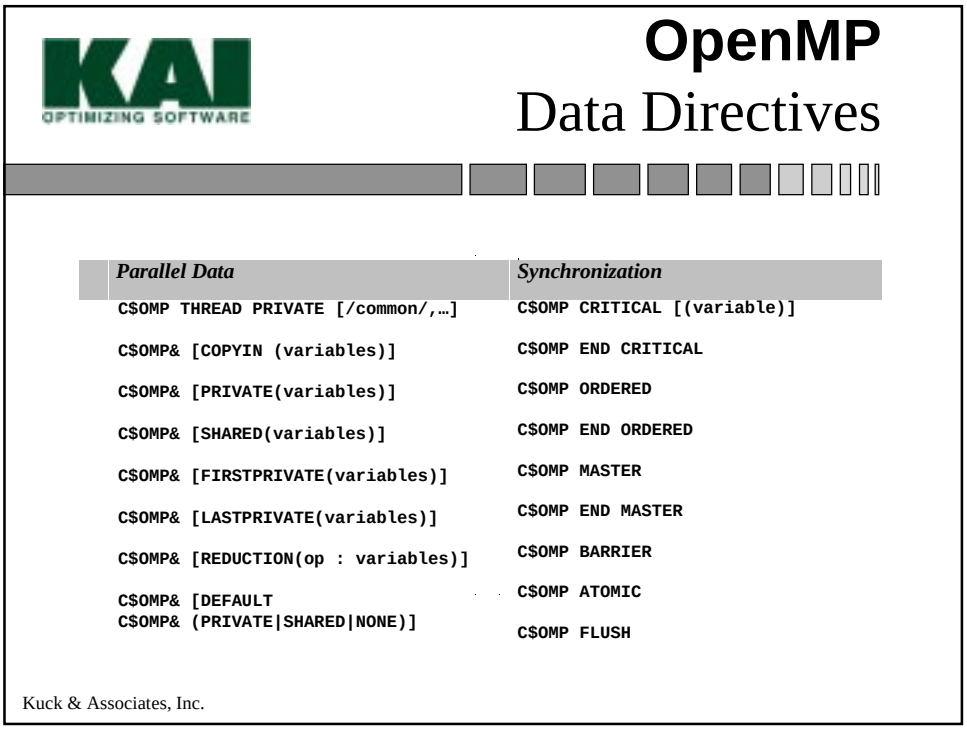
OpenMP
Data Directives
Parallel Data
C$OMP THREAD PRIVATE [/common/,…]
C$OMP& [COPYIN (variables)]
C$OMP& [PRIVATE(variables)]
C$OMP& [SHARED(variables)]
C$OMP& [FIRSTPRIVATE(variables)]
C$OMP& [LASTPRIVATE(variables)]
C$OMP& [REDUCTION(op : variables)]
C$OMP& [DEFAULT
C$OMP& (PRIVATE|SHARED|NONE)]
Synchronization
C$OMP CRITICAL [(variable)]
C$OMP END CRITICAL
C$OMP ORDERED
C$OMP END ORDERED
C$OMP MASTER
C$OMP END MASTER
C$OMP BARRIER
C$OMP ATOMIC
C$OMP FLUSH
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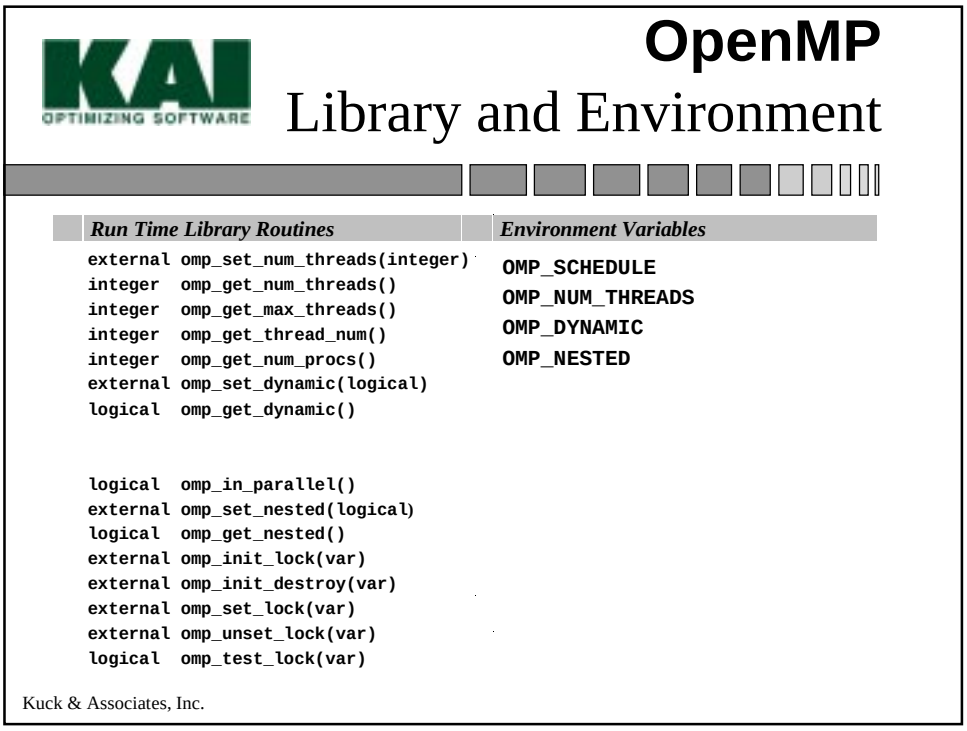
OpenMP
Library and Environment
Run Time Library Routines
external omp_set_num_threads(integer)
integer omp_get_num_threads()
integer omp_get_max_threads()
integer omp_get_thread_num()
integer omp_get_num_procs()
external omp_set_dynamic(logical)
logical omp_get_dynamic()
logical omp_in_parallel()
external omp_set_nested(logical)
logical omp_get_nested()
external omp_init_lock(var)
external omp_init_destroy(var)
external omp_set_lock(var)
external omp_unset_lock(var)
logical omp_test_lock(var)
Environment Variables
OMP_SCHEDULE
OMP_NUM_THREADS
OMP_DYNAMIC
OMP_NESTED
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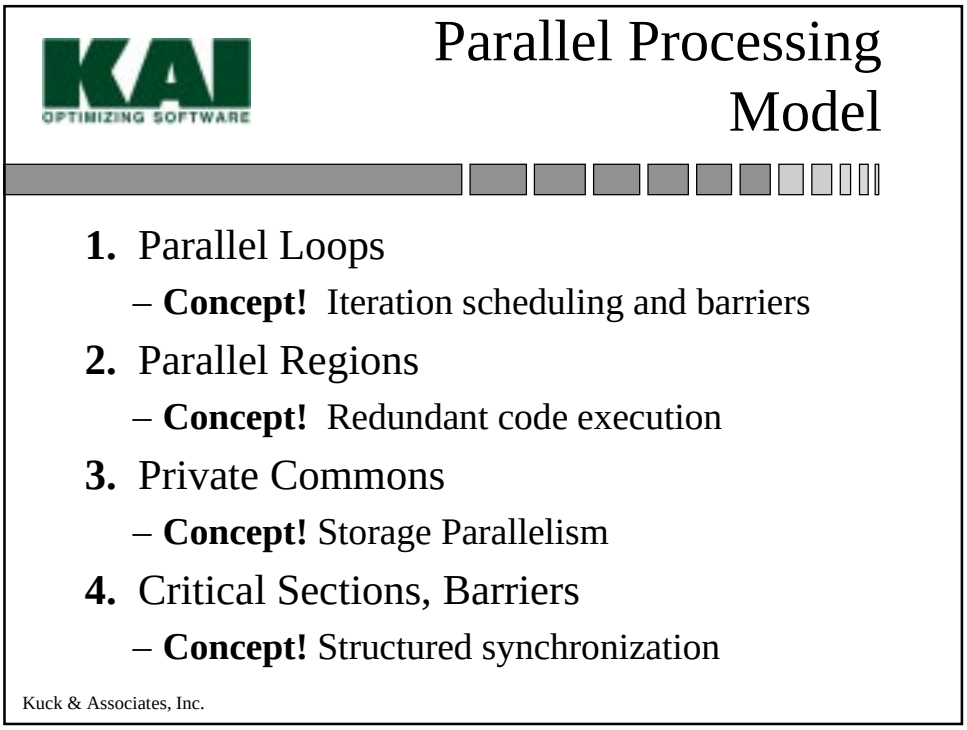
Parallel Processing Model
1. Parallel Loops
– Concept! Iteration scheduling and barriers
2. Parallel Regions
– Concept! Redundant code execution
3. Private Commons
– Concept! Storage Parallelism
4. Critical Sections, Barriers
– Concept! Structured synchronization
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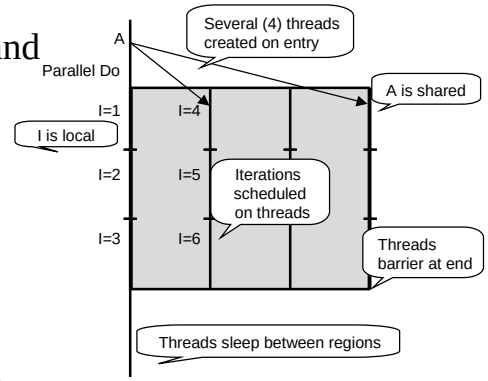
Parallel Loop Model

- Note threads, shared and private variables.

```
      program example
c$omp parallel do
c$omp& shared(A)
c$omp& private(I)
      do I=1,100
       A(I) = ...
      end do
c$omp end parallel do
      end
```



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Parallel Region Model

- Note "redundant" code

All threads execute same code

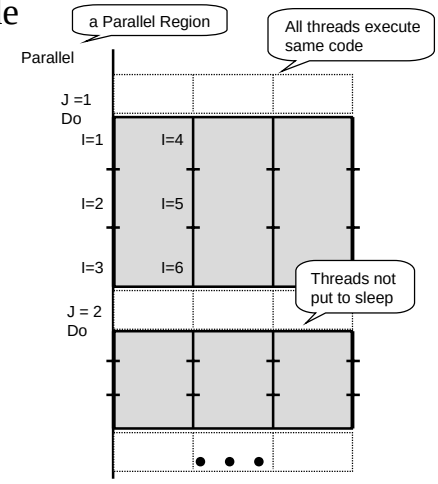
Threads execute "different" code

All threads execute same code

```
c$omp parallel
    do j =1,jconverg

c$omp do
      do i=ilb,iub
        ...
      end do

    end do
c$omp end parallel
```



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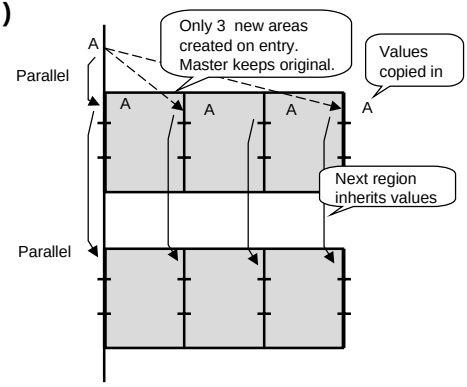
Parallel Storage Model

- Note THREAD PRIVATE

```
c$omp threadprivate(/A/)
   common /A/ data(100)
c$omp parallel
c$omp& copyin(/A/)
    ...
c$omp end parallel

c$omp parallel
c$omp end parallel
```



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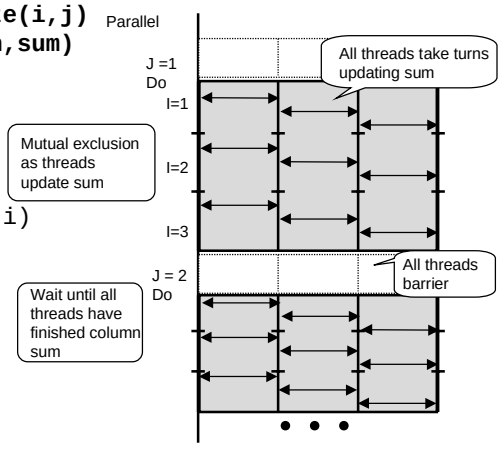
Parallel Synchronization Model

- Critical section and Barrier

```
c$omp parallel private(i,j)
c$omp& shared(a,b,m,n,sum)
      do 20 i=1,n
       sum = 0
c$omp  do
       do 10 j=1,m
c$omp   critical
         sum=sum+a(j,i)
c$omp   end critical
10     continue
c$omp  barrier
       b(i) = sum
20    continue
c$omp end parallel
```



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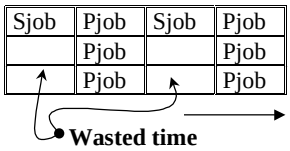
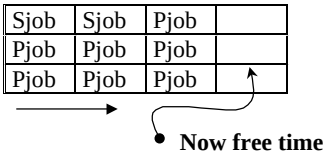
OpenMP Feature Dynamic Threads

Without Dynamic Threads



With Dynamic Threads



- With Static Threads
  - Request 3 threads
  - Get exactly 3 threads
- With Dynamic Threads
  - Request 3 threads
  - Get 3 threads **if available**
- Your job gets done faster **and** your colleagues too
- Avoids over allocating processors

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Experience Learned with Directive Programs

- Ideal for directives
  - Model 1: Fork, share work, join and repeat
- Parallelism in whole program didn't work
  - Model 2: Fork once - barrier when needed
- OpenMP has added orphaned directives

Model 2: **Before** OpenMP

```
c$par parallel
   myid = mpptid()
   ichunk = isize / mppnth()
   mywork = ichunk * myid
   call
   simul8(myid,mywork,ichunk)
c$par end parallel
   ...
   subroutine simul8(myid,
                     mywork, ichunk)
   do i=mywork,mywork+ichunk
    call realwork
   end do
c$par barrier
   end
```

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OpenMP Feature Orphaned Directives

- Now directives don't have to be in the same subroutine
- Removes need for:
  - Explicit scheduling
  - Passing scheduling arguments
  - Explicit barriers
- Dynamic binding

Model 2: **After** OpenMP

```
c$omp parallel
   call simul8(normal args)
c$omp end parallel
   ...
   subroutine simul8(args)
c$omp do schedule(static)
   do i=0,isize
    call realwork
   end do
   end
```

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OpenMP IF clause Reduce parallel overhead

- Optional IF clause for PARALLEL or PARALLEL DO directive

```
c$omp parallel do if(n .GE. 10*numcpus)
```

  - If true, execute region on multiple processors
  - If false, execute region on single processor
- Identify short parallel regions that may slow you down
- Select best loop in nested loops at runtime

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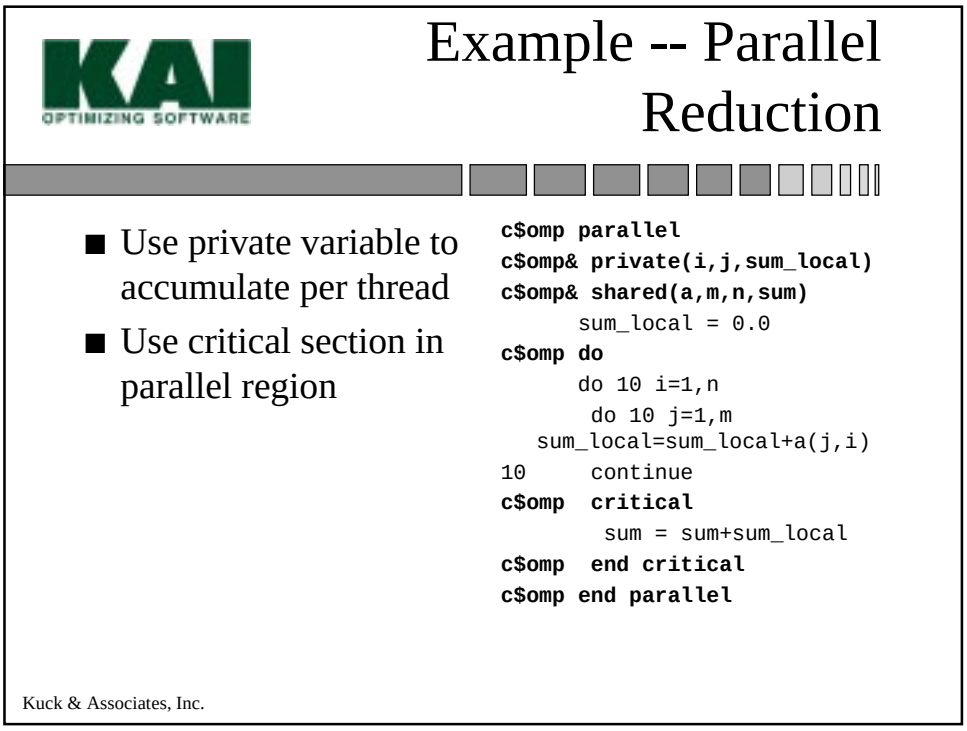
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Example -- Parallel Reduction
Use private variable to accumulate per thread
Use critical section in parallel region
c$omp parallel
c$omp& private(i,j,sum_local)
c$omp& shared(a,m,n,sum)
sum_local = 0.0
c$omp do
do 10 i=1,n
do 10 j=1,m
sum_local=sum_local+a(j,i)
10 continue
c$omp critical
sum = sum+sum_local
c$omp end critical
c$omp end parallel
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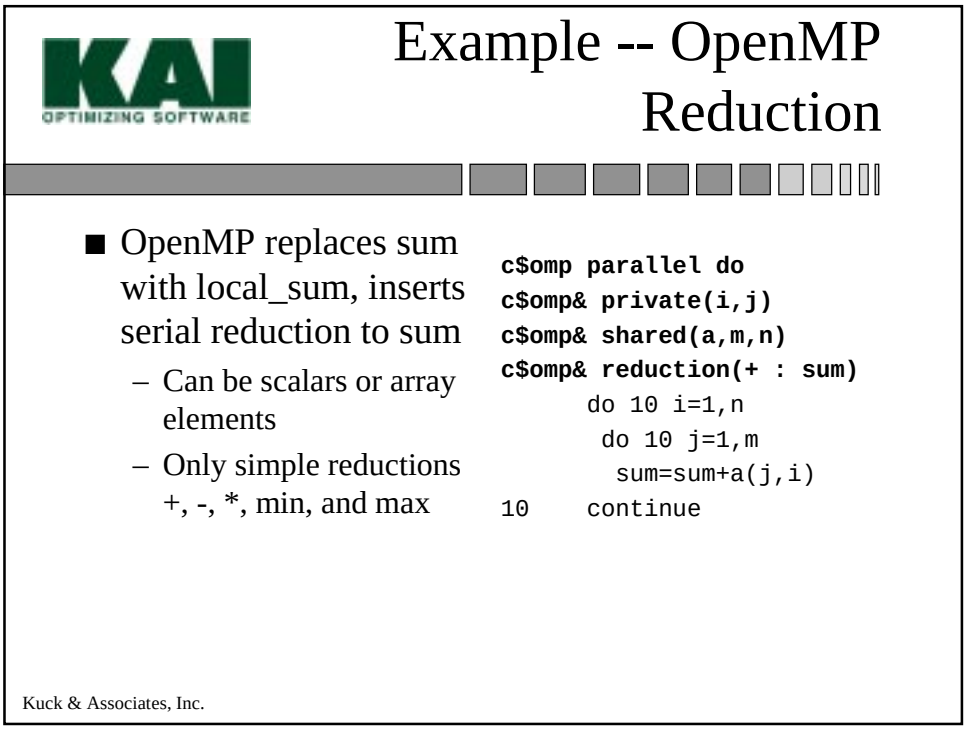
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Example -- OpenMP Reduction
OpenMP replaces sum with local_sum, inserts serial reduction to sum
– Can be scalars or array elements
– Only simple reductions +, -, *, min, and max
c$omp parallel do
c$omp& private(i,j)
c$omp& shared(a,m,n)
c$omp& reduction(+ : sum)
do 10 i=1,n
do 10 j=1,m
sum=sum+a(j,i)
10 continue
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KPTS + OpenMP = Parallel Software Engineering

- Performance --
  - Meets or beats all modes on scalability
- Productivity --
  - Much easier to use than other modes
- Quality --
  - Enables parallelism validation for first time
- Standards --
  - Defacto becoming fact

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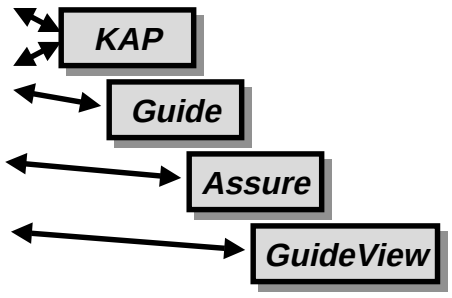
OpenMP Parallel Software Engineering with ***KPTS***

- Steps in Parallelizing an Application
  - **A**nalyze
  - **R**estructure
  - **T**est
  - **I**mprove
  - **Q**/A



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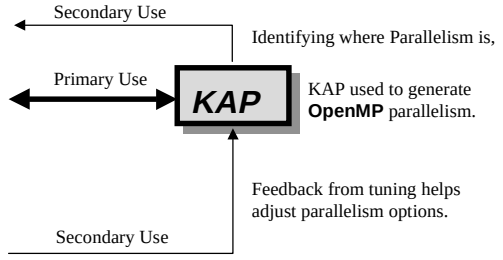
What is KAP

- ***KAP*** restructures to **OpenMP** parallelism
  - **A**nalyze
  - **R**estructure
  - **T**est
  - **I**mprove
  - **Q**/A



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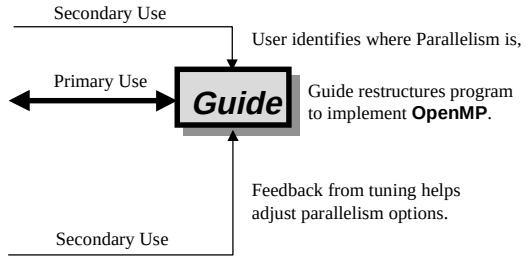
What is Guide

- ***Guide*** implements **OpenMP** parallelism
  - **A**nalyze
  - **R**estructure
  - **T**est
  - **I**mprove
  - **Q**/A



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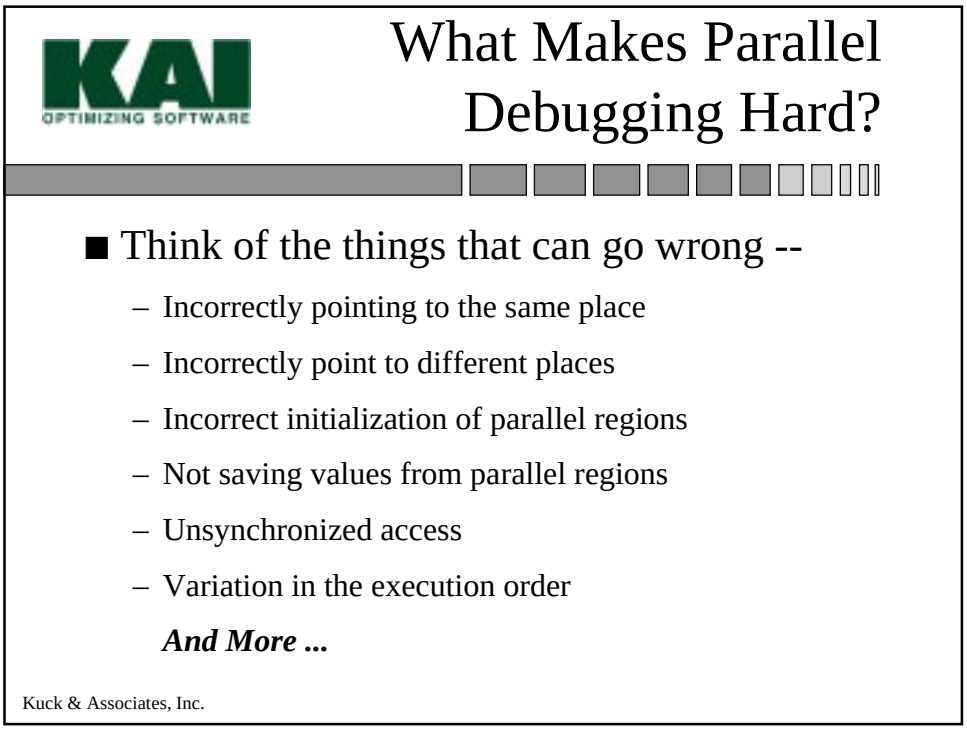
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What Makes Parallel Debugging Hard?
■ Think of the things that can go wrong --
– Incorrectly pointing to the same place
– Incorrectly point to different places
– Incorrect initialization of parallel regions
– Not saving values from parallel regions
– Unsynchronized access
– Variation in the execution order
And More ...
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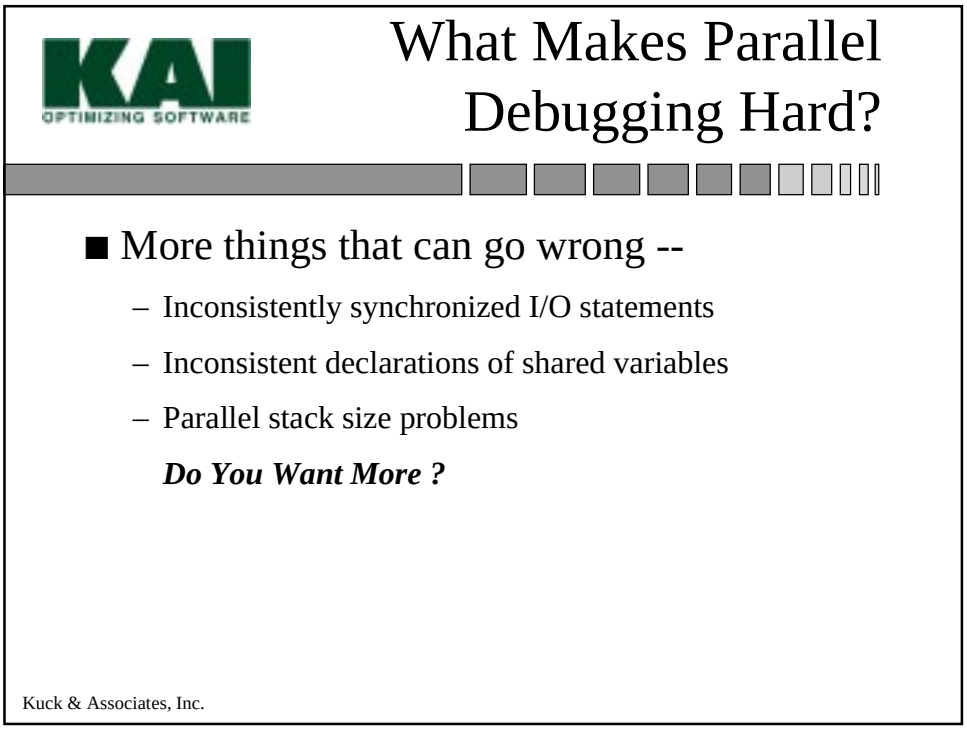
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What Makes Parallel Debugging Hard?
■ More things that can go wrong --
– Inconsistently synchronized I/O statements
– Inconsistent declarations of shared variables
– Parallel stack size problems
Do You Want More ?
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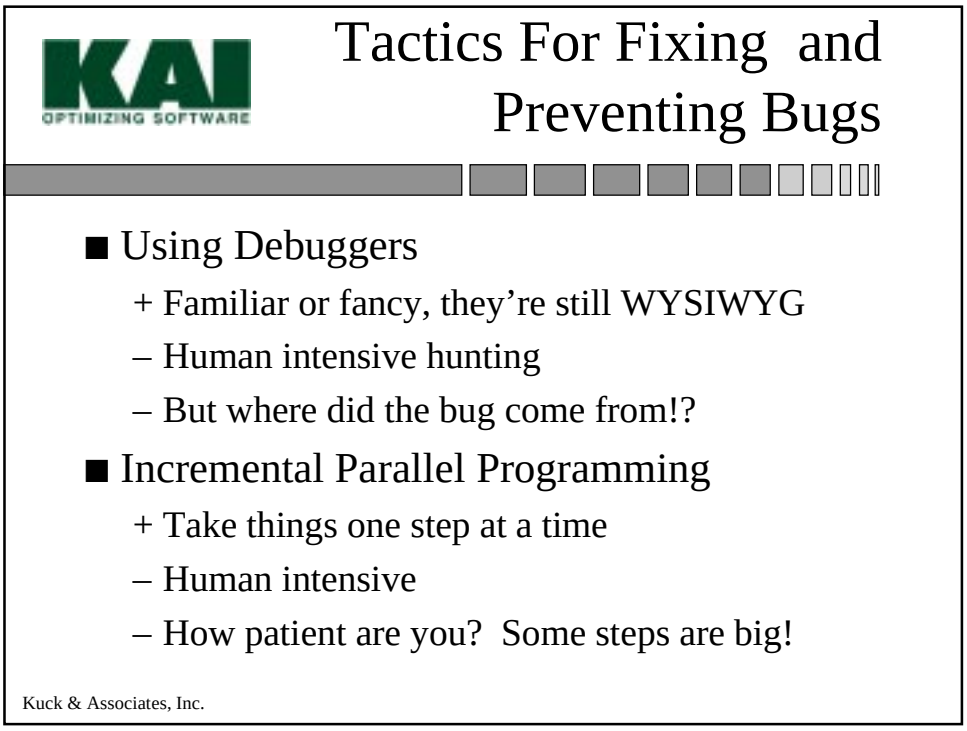
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Tactics For Fixing and Preventing Bugs
■ Using Debuggers
+ Familiar or fancy, they're still WYSIWYG
– Human intensive hunting
– But where did the bug come from!?
■ Incremental Parallel Programming
+ Take things one step at a time
– Human intensive
– How patient are you? Some steps are big!
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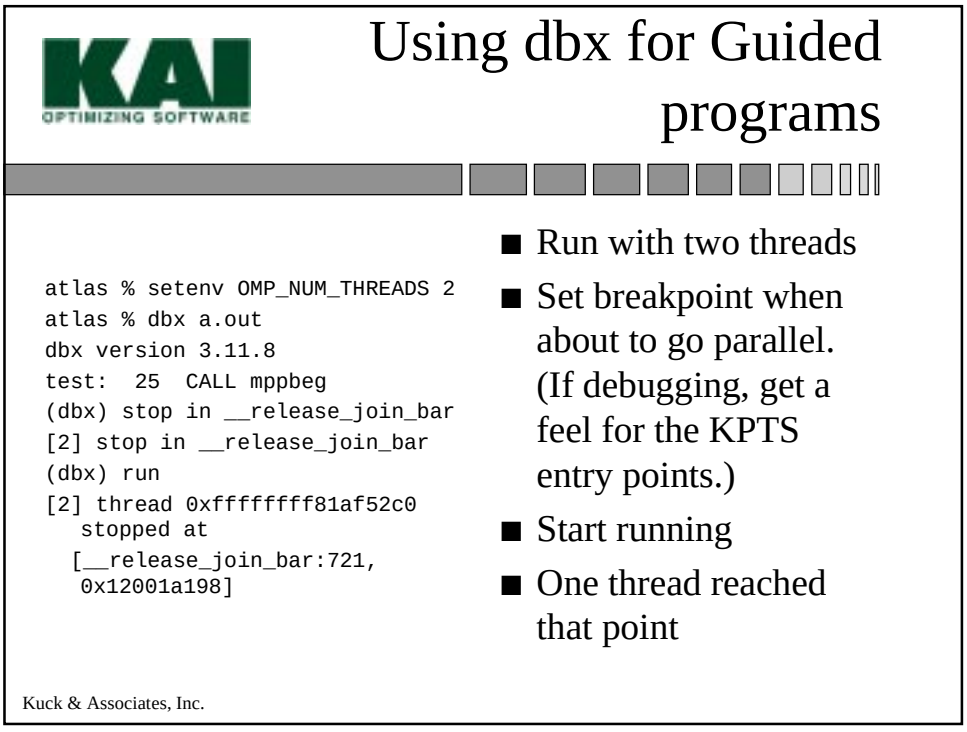
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Using dbx for Guided programs
atlas % setenv OMP_NUM_THREADS 2
atlas % dbx a.out
dbx version 3.11.8
test: 25 CALL mppbeg
(dbx) stop in __release_join_bar
[2] stop in __release_join_bar
(dbx) run
[2] thread 0xffffffff81af52c0
stopped at
[__release_join_bar:721,
0x12001a198]
■ Run with two threads
■ Set breakpoint when about to go parallel. (If debugging, get a feel for the KPTS entry points.)
■ Start running
■ One thread reached that point
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Using dbx for Guided programs

```
(dbx) tstack
Thread 0xffffffff81af52c0:
>  0 __kmp_release_join_barrier() ...
   1 mppfrk_() ["kmp_fork.c":325, ...
   2 test() ["x.cmp.f":29,
   0x120019754]
   3 main() ["for_main.c":203, ...
Thread 0xffffffff81af4780:
>  0 __sigaction(0x0, 0x0, 0x0, 0x0)
   1 cma__sig_thread_init(
   0x3ff8103e15 ...
   2 cma__thread_base(0x0, 0x0, 0x0)
(dbx) tset 0xffffffff81af4780
thread 0xffffffff81af4780 stopped at
   ...
(dbx) continue
```

- Inquire what threads are doing with tstack
- Switch to other thread with tset
- Continue running

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Better Tactic For Bugs

- ***Assure*** systematically finds Communication Leaks
  - + Identifies source of bug as well
  - + Finds non-deterministic errors
  - + Trades computer time for human time

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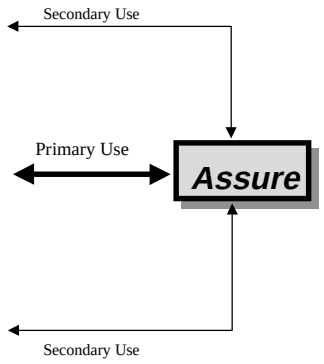
What is Assure

- ***Assure*** for validating **OpenMP**
  - **A**nalyze
  - **R**estructure
  - **T**est
  - **I**mprove
  - **Q**/A



Input:
Program with **OpenMP** directives; test data.

Output:
Report of communication leaks.

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Why isn't this automated? (Ans: It is. E.g., ***Assure***.)

- Guide provides compile time diagnostics
  - Limits: subroutine being compiled and heuristic
- What is Assure?
  - *Validates* parallel programs
  - Missing or incorrect scoping is *invalid*
- What does Assure do?
  - Simulates parallel run
  - Finds *communication leaks*!

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What Is Parallel Validation?

- ***Assure*** identifies *incorrect behavior for parallel program*
- Define correct behavior? ***Assure*** uses --
  - Parallel program and a provided data-set
- When validated, a program is valid --
  - For any number of processors at runtime
  - For all execution timing variations
  - Across supported platforms

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Verifying Storage Class Choice

- Misclassified x and y as shared

```
01:  subroutine dsq(a, b, c, n)
02:c$omp parallel do private(i)
03:c$omp& shared(a,b,c,n,x,y)
04:  do i = 1,n
05:   x = a(i) - b(i)
06:   y = b(i) + a(i)
07:   c(i) = x * y
08:  end do
```

- Assure report:

Storage conflicts in PARALLEL DO, DSQ/2 (dsq.f):

Conflict Type	Source Symbol	Source - Sink
Read -> Write	X	DSQ/7 - 5
Read -> Write	Y	DSQ/7 - 6
Write -> Write	X	DSQ/5
Write -> Write	Y	DSQ/6

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Verifying Storage Class Choice

- Misclassified a and b as private

```
01:  subroutine dsq(a, b, c, n)
02:c$omp parallel do shared(c, n)
03:c$omp& private(i, a, b, x, y)
04:  do i = 1,n
05:   x = a(i) - b(i)
06:   y = b(i) + a(i)
07:   c(i) = x * y
08:  end do
```

- Assure report:

Errors in PARALLEL DO, DSQ/2 (dsq.f):

Error: DSQ/5 (dsq.f): uninitialized read of PRIVATE symbol 'B' in PARALLEL DO

Error: DSQ/5 (dsq.f): uninitialized read of PRIVATE symbol 'A' in PARALLEL DO

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Assure Example

- Invalid data bug:

```
      do 10 n=1,1000
 10    A(n) = 0.0
 c$omp parallel do private(B,i,j)
 c$omp& shared(A,m,a1,a2,b1,b2)
       do i=1,m
        do 20 j=a1(i),a2(i)
20       A(j) = (expression)

        do 30 j=b1(i),b2(i)
30       B(j) = (Reference to A(j))
       end do

       print *,B
```

Valid Data -- m=4

i	a1	a2
1	1	3
2	4	6
3	7	9
4	10	12

i	b1	b2
1	1	3
2	4	6
3	7	9
4	10	12

INvalid Data -- m=4

i	a1	a2
1	1	3
2	4	6
3	7	9
4	10	12

i	b1	b2
1	2	**4**
2	5	**7**
3	8	**10**
4	11	**13**

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Assure Example

- Invalid data bug:

```
01:      do 10 i=1,20
02: 10    A(i) = 0.0
03:c$omp parallel do private(B,i,j)
04:c$omp& shared(A,a1,a2,b1,b2,m)
05:      do i=1,m
06:       do 20 j=a1(i),a2(i)
07: 20     A(j) = (Expression)
08:       do 30 j=b1(i),b2(i)
09: 30     B(j) = (Func of A(j))
10:      end do
11:      do 40 i=1,20
12: 40     print *, B(i)
```

- Assure Report:

Errors in ROUTINE, ITER/1 (iter.f):

Error: ITER/9 (iter.f): PRIVATE symbol 'B' referenced outside parallel construct as 'B' in ITER/12

Storage conflicts in PARALLEL DO, ITER/16 (iter.f):

Conflict Type	Source Symbol	Source - Sink Routine/Line
Write -> Read	A	ITER/7 - 9

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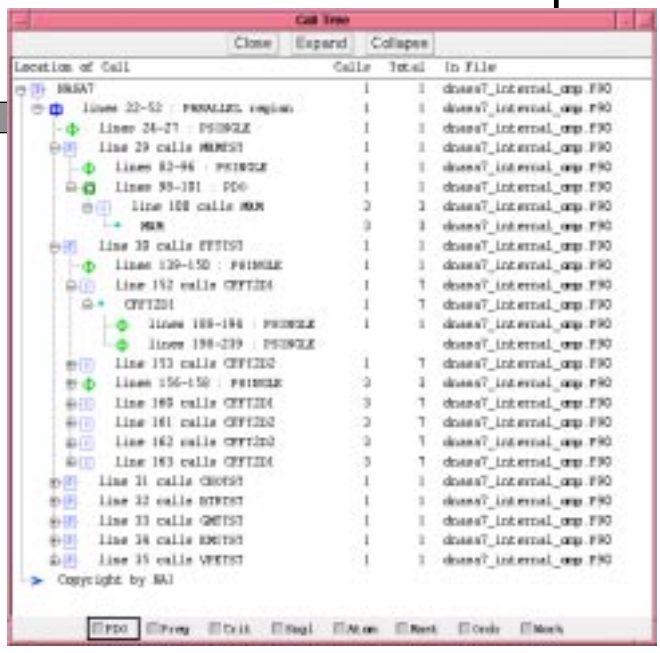
AssureView: Call Graph



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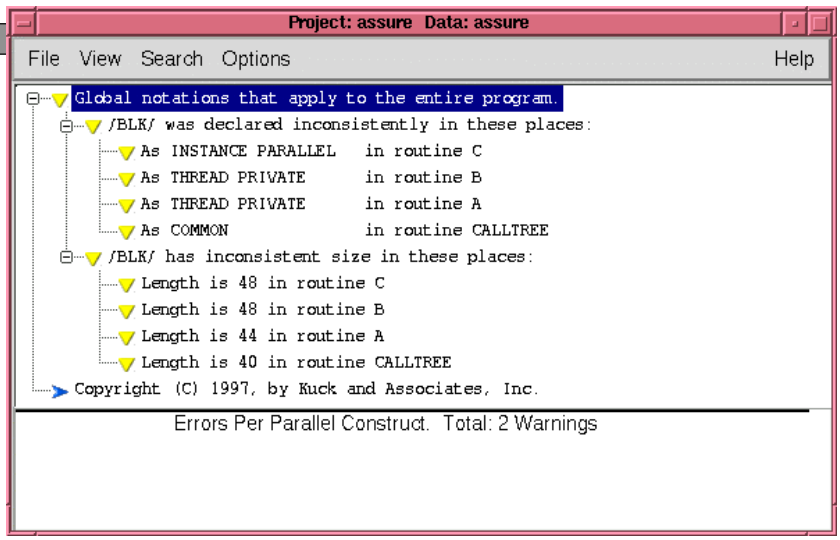
AssureView: Common Mismatch



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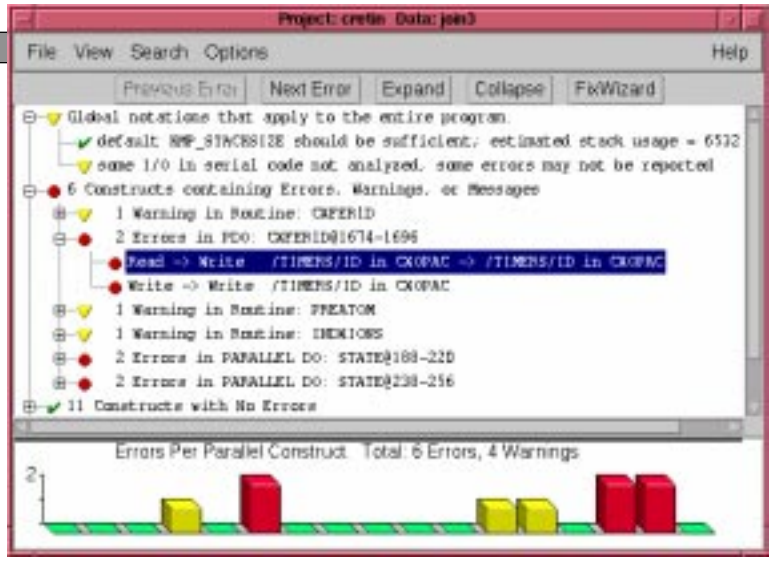
AssureView: Errors



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AssureView:Source

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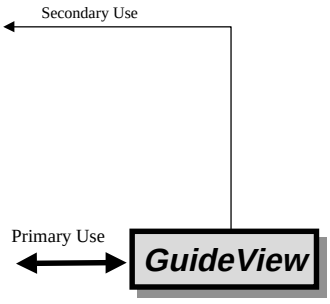
What is GuideView

- ***GuideView*** visualizes **OpenMP**
  - **A**nalyze
  - **R**estructure
  - **T**est
  - **I**mprove
  - **Q**/A



Input:
Program with **OpenMP** directives; test data.

Function:
Navigate complex problem down to performance problems

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Example Profile

Each sample covers 4.00 byte(s) for 8.3e-06% of 11743.0342 seconds

%time	seconds	cum %	cum sec	procedure (file)
8.5	1003.0098	8.5	1003.01	proj_slv_node_on_mr_seg_
4.7	548.3232	17.9	2102.68	shell_force_el_pl_4p_
4.4	522.3145	22.4	2624.99	pkshell_egy_el_pl_v__
3.8	450.5781	26.2	3075.57	shell_lam_stress_pl_3d_
3.3	382.9053	40.2	4718.43	pkcalc_node_vel__
3.2	372.4639	43.4	5090.90	pkcalc_node_accel__
3.1	365.8145	46.5	5456.71	shell_stress_el_pl_
2.6	306.9453	60.8	7144.42	pkcontact_node_trial_vel_posn_1_
2.4	276.1680	63.2	7420.58	trans_lvecs_to_gvecs_
2.3	270.2891	65.5	7690.87	spin_wait_join_barrier

. . .

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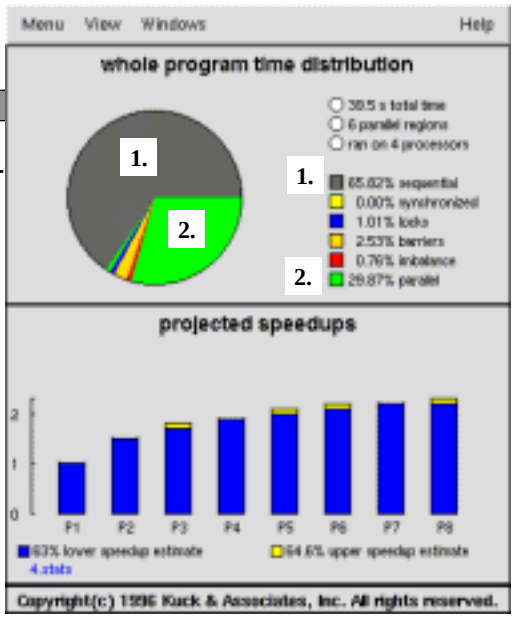
GuideView adds focus

- Visualize the performance report
- Pie Chart --
  - Percent parallel
  - Overhead
    - » Locks
    - » Barriers
    - » Imbalance
- Bar Chart --
  - Amdahl's Law



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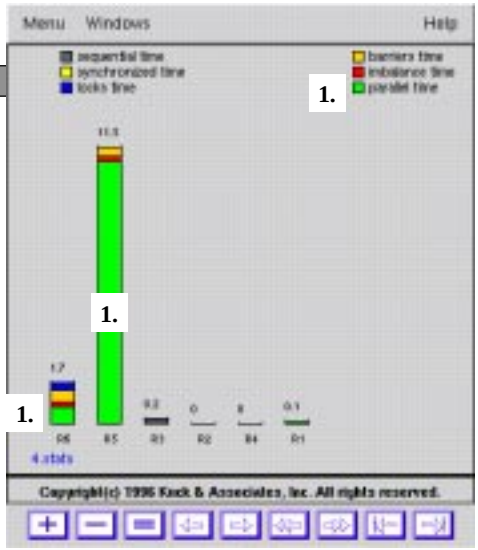
GuideView adds focus

- Parallel regions
- Sorted by --
  - Overhead
  - Time
- Compare --
  - Parallel time
  - Synched time
  - Lock time
  - Barrier time



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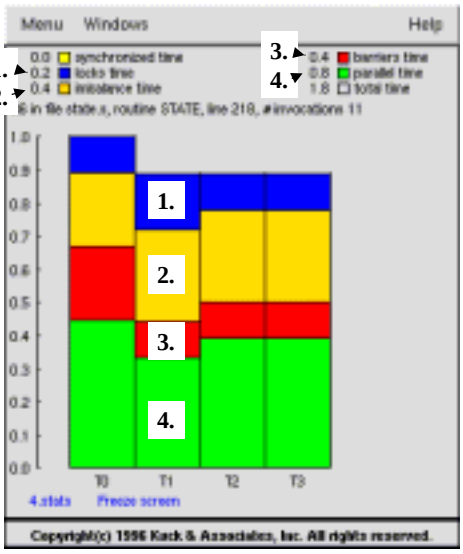
GuideView adds focus

- Per Region
  & Per Thread
- High Barrier Time!
- Load Imbalance Possible

(Note: this is a small run)



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DGauss Performance

	Intel Pentium Pro (200Mhz)			Cray J90
	P=1	**P=4**	**Speedup**	**P=1**
Job 1	54	20	2.7	25
Job 2	491	194	2.5	180
Job 3	3241	1256	2.6	912
Job4	13362	5700	2.3	3840

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MM5 Performance

	Small Problem		Large Problem	
	Digital Alpha (400Mhz)		Digital Alpha (400Mhz)	Intel Pentium Pro (200Mhz)
	Unix	**NT**	**NT**	**NT**
Serial	1.0	1.0		1.0
P=1	1.0 (760)	1.0 (701)	1.0 (14272)	1.0 (47834)
P=2	1.87	1.82	1.90	1.83
P=3	2.59	2.46	2.72	2.44
P=4	3.25 (234)	3.03 (233)	3.48 (4098)	2.90 (16489)

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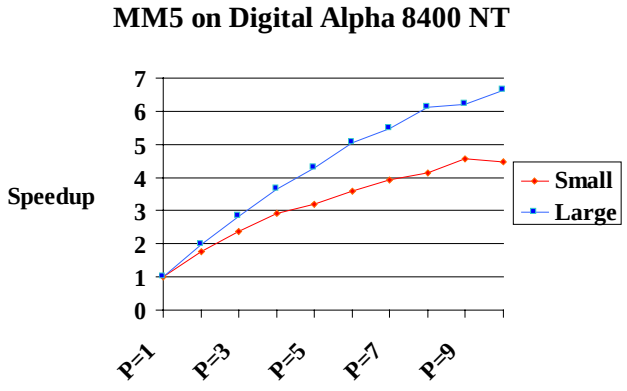
MM5 Scalability



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Conclusion

http://www.openmp.org

- Parallel Software Engineering needs to be addressed to produce quality applications.
- OpenMP solves the portability problem.
- The KAP/Pro Toolset for OpenMP is available now!

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