



Tri-hybrid Computational Fluid Dynamics on DoE's Cray XK7, Titan.

Aaron Vose, Brian Mitchell, and John Levesque
CUG - 5/8/2014



Hybrid CFD - Overview

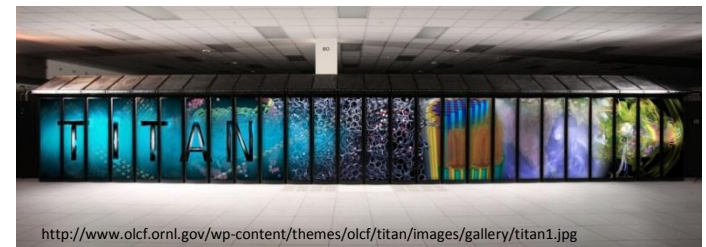
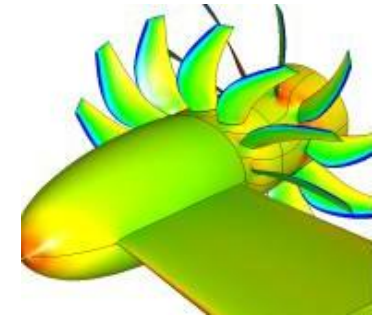
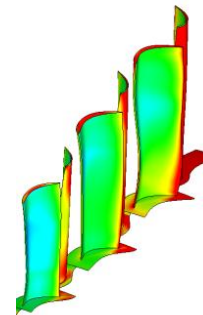
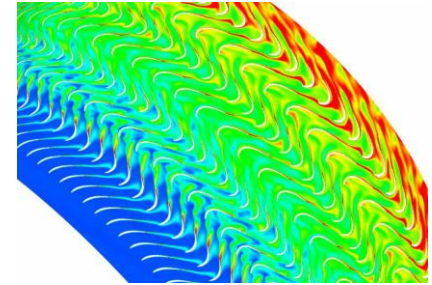
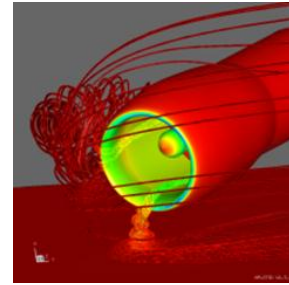
- Introduction to GE's TACOMA.
- OpenMP porting effort.
 - Lessons learned.
- OpenACC porting effort.
 - Lessons learned.
- Performance results.

Expressing Underlying Algorithmic Parallelism



Turbomachinery CFD @ GE

- Essential to the design process.
- Jet engines, gas turbines, steam turbines, and more.
- 10's of cores → >10K cores.
- US National Lab supercomputers prove computational technology.





Hybrid CFD - TACOMA

- Computational Fluid Dynamics (CFD) code.
 - Used heavily for turbomachinery airfoil design
 - 2nd order accurate in time and space.
 - Finite-volume, block-structured, compressible flow solver.
 - Stability achieved via JST^[1].
 - Convergence accelerated with pseudo-time marching and multi-grid.

[1] JAMES, A., SCHMIDT, W., AND TURKEL, E. "Numerical solution of the euler equations by finite volume methods using runge-kutta time-stepping schemes." AIAA (1981).



Hybrid CFD - OpenMP Porting

- Express existing loop-level parallelism with OMP directives.
- Port to OpenMP before OpenACC.
 - OpenACC can reuse most OMP scoping.
 - OMP is easier; data motion can be ignored.
- Modify loops to expose more of underlying algorithms' parallelism.



Hybrid CFD - Algo. Parallelism

```
do k=1,n3
  do j=1,n2
    do i=1,n1
      df(1:3) = dflux(i,j,k)
      R(i,j,k) += df(1) +
                df(2) +
                df(3)
      R(i-1,j,k) -= df(1)
      R(i,j-1,k) -= df(2)
      R(i,j,k-1) -= df(3)
    end do
  end do
end do
```

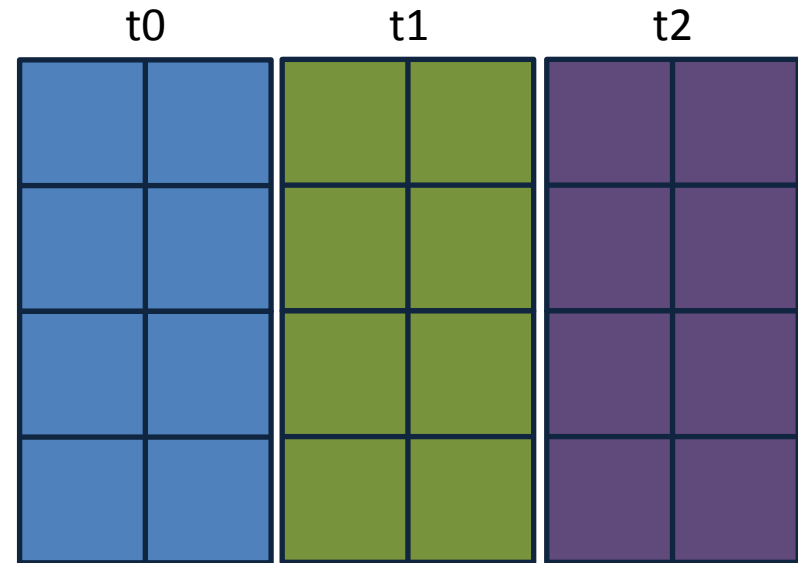


Hybrid CFD - Algo. Parallelism



```
do k=1,n3
  do j=1,n2
    do i=1,n1
      df(1:3) = dflux(i,j,k)
      R(i,j,k) += df(1) +
                df(2) +
                df(3)
      R(i-1,j,k) -= df(1)
      R(i,j-1,k) -= df(2)
      R(i,j,k-1) -= df(3)
    end do
  end do
end do
```

OpenMP





Hybrid CFD - Algo. Parallelism

```

do k=1,n3
  do j=1,n2
    do i=1,n1
      df(1:3) = dflux(i,j,k)
      R(i,j,k) += df(1) +
                df(2) +
                df(3)

      R(i-1,j,k) -= df(1)
      R(i,j-1,k) -= df(2)
      R(i,j,k-1) -= df(3)
    end do
  end do
end do

```

```

do k=1,n3
  do j=1,n2
    do i=1,n1
      df(i,j,k,1:3) = dflux(i,j,k)
    end do
  end do
end do

```

OpenACC

```

do k=1,n3
  do j=1,n2
    do i=1,n1
      R(i,j,k) += df(i,j,k,1) +
                 df(i,j,k,2) +
                 df(i,j,k,3)

      R(i,j,k) -= df(i+1,j,k,1) +
                 df(i,j+1,k,2) +
                 df(i,j,k+1,3)
    end do
  end do
end do

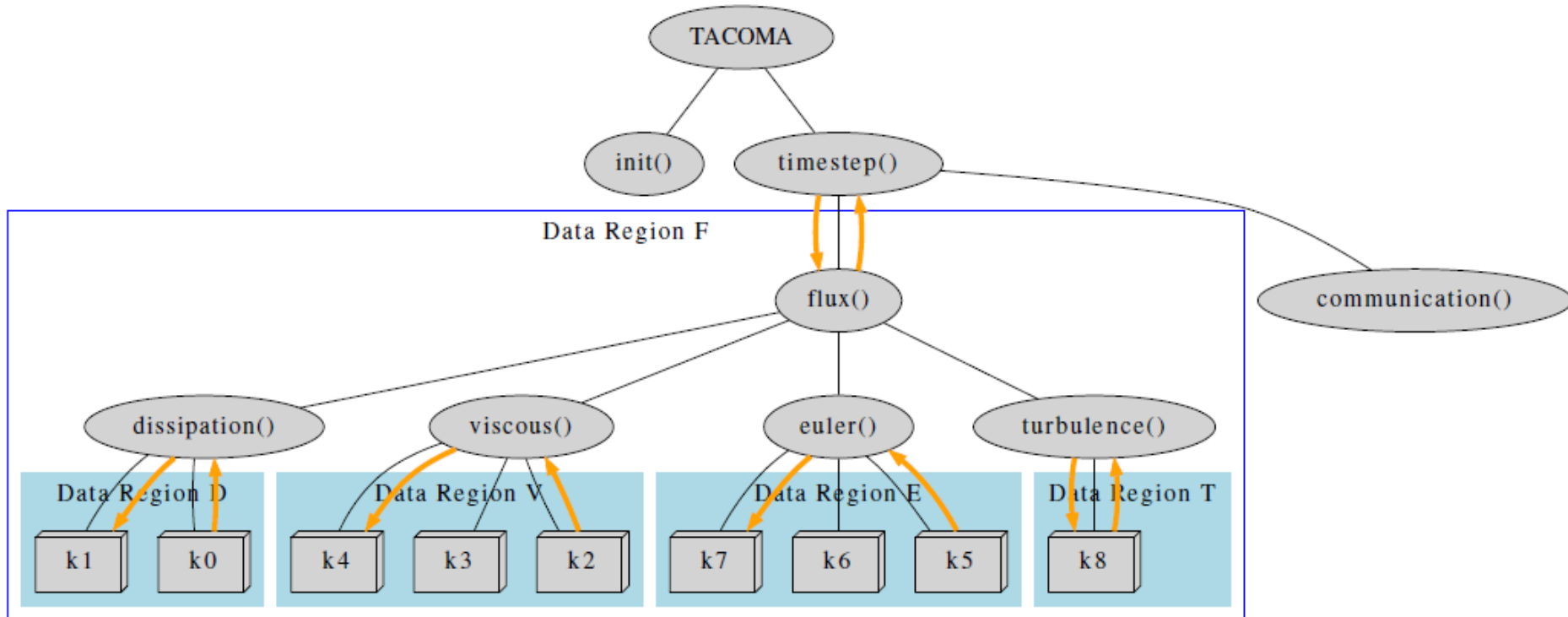
```




Hybrid CFD - OpenACC Porting

- Identify candidate loops:
 - Check loops' trip/iteration count (CrayPAT).
- Add OpenACC directives / Optimize Kernels:
 - Check compiler listing for proper vectorization.
 - Ignore data motion (best performed once kernels are done and have known data requirements).
- Finally, optimize device \leftrightarrow host data motion.

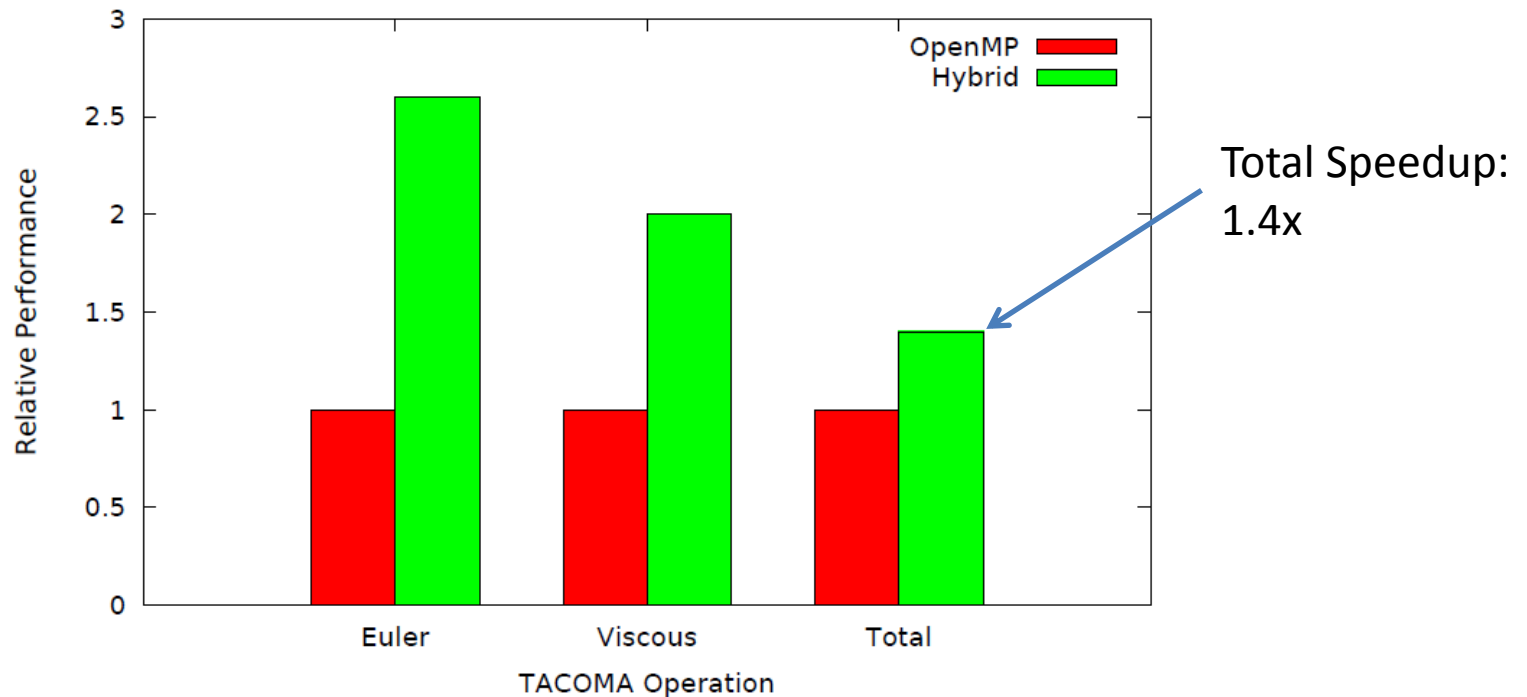
Hybrid CFD - OpenACC Data



- Create OpenACC data regions:
 - Keep data on the GPU device as long as possible.



Hybrid CFD - Performance Results



- **MPI+OpenMP** vs. **MPI+OpenMP+OpenACC.**



Hybrid CFD - Conclusion

- Lessons learned:
 - Port to OpenMP before OpenACC.
 - Reuse scoping work.
 - Optimize OpenACC data motion last.
 - Perform bottom-up, hierarchical data optimization.
 - Express underlying algorithm's parallelism.
 - Don't limit parallelism by existing implementation.
- TACOMA's OpenACC achieves 1.4x speedup.



Hybrid CFD - Legal

- **Acknowledgement:** This research used resources of the OLCF at ORNL, which is supported by the Office of Science of the U.S. DoE under Contract No. DE-AC05-00OR22725.
- **Safe Harbor Statement:** This presentation may contain forward-looking statements that are based on our current expectations. Forward looking statements may include statements about our financial guidance and expected operating results, our opportunities and future potential, our product development and new product introduction plans, our ability to expand and penetrate our addressable markets and other statements that are not historical facts. These statements are only predictions and actual results may materially vary from those projected. Please refer to Cray's documents filed with the SEC from time to time concerning factors that could affect the Company and these forward-looking statements.
- **Legal Disclaimer:** Information in this document is provided in connection with Cray Inc. products. No license, express or implied, to any intellectual property rights is granted by this document. Cray Inc. may make changes to specifications and product descriptions at any time, without notice. All products, dates and figures specified are preliminary based on current expectations, and are subject to change without notice. Cray hardware and software products may contain design defects or errors known as errata, which may cause the product to deviate from published specifications. Current characterized errata are available on request. Cray uses codenames internally to identify products that are in development and not yet publically announced for release. Customers and other third parties are not authorized by Cray Inc. to use codenames in advertising, promotion or marketing and any use of Cray Inc. internal codenames is at the sole risk of the user. Performance tests and ratings are measured using specific systems and/or components and reflect the approximate performance of Cray Inc. products as measured by those tests. Any difference in system hardware or software design or configuration may affect actual performance. The following are trademarks of Cray Inc. and are registered in the United States and other countries: CRAY and design, SONEXION, URIKA, and YARCDATA. The following are trademarks of Cray Inc.: ACE, APPRENTICE2, CHAPEL, CLUSTER CONNECT, CRAYPAT, CRAYPORT, ECOPHLEX, LIBSCI, NODEKARE, THREADSTORM. The following system family marks, and associated model number marks, are trademarks of Cray Inc.: CS, CX, XC, XE, XK, XMT, and XT. The registered trademark LINUX is used pursuant to a sublicense from LMI, the exclusive licensee of Linus Torvalds, owner of the mark on a worldwide basis. Other trademarks used in this document are the property of their respective owners.