

#### Turbomachinery R&D Acceleration using Titan

R. Srinivasan Aero/Thermodynamic Engineer Dresser-Rand

GTC 2015, San Jose, CA



# Outline Background Software Developments Application Strategy Titan focused development Applications • Open Science Turbomachinery R&D Conclusions



## BACKGROUND



© Copyright 2009

3

#### Background

- Partnership with Oak Ridge National Laboratory's Leadership Computing Facility
- Utilize large scale DoE hardware at OLCF to improve development time of new turbomachinery designs
- Commercial software package
  - The Fine/Turbo suite
    - CFD tools for high fidelity turbomachinery analysis
    - Advanced features for fast, high fidelity simulations
- Software development program
  - Jointly funded
- Time-allocation through DD and ALCC



#### Background – Software Developments

- Virtual decomposition of the multiblock grid
- Distributed memory parallel computing with MPI
- I/O improvements
- Parallelization of turbomachinery related BC
- Efficient scalability with up to 4000 compute processes
- Ongoing effort

DRESSER RAND





## Application Strategy

- Turbomachinery R&D
- Time frame for design and development
- Parametric optimization
- Ensemble runs for database generation
- Design refinement



## TITAN FOCUSSED DEVELOPMENT



© Copyright 2009

7

## GPU Strategy

Utilization of new GPU hardware on Titan

- Software Limitations
- Industrial Limitations
- Cost of rewriting the solver
- Investigated alternatives
  - Selection of appropriate code module for acceleration



#### **GPU Accelerated Module**

- Advanced residual smoothing algorithm, bringing a level of implicitness to the time integration solver
- Permits the use of high CFL numbers

DRESSER RAND

- Yields a drastic decrease in the number of iterations needed for convergence (~4x)
- Time per iteration is increased due to the additional module arithmetic (~2x)
- Attractive candidate for threaded execution, either on CPU or
  GPU
  CPU booster
  MGS 1111 CE 100
  MGS 1234 CE 1



# Hardware and Software Considerations

- Titan nodes are equipped with PCIe 2.0
- Each node contains 16 CPU cores, all of which will simultaneously transfer data to a single GPU
- Bandwidth in/out of the GPU is a bottleneck
- GPU memory is also a limitation for larger computations
- OpenACC programming model
  - Directive based approach for usability and ease of maintainance



#### Test Case Performance

- Positive speedup of 1.25x observed during execution of typical sample model
- Speedup dependence on internal boundary conditions
- Peak speedup of 1.7x
  observed for conformal
  BC model



Typical sample speedup of 1.25x, maximum of 1.7x.





**IO** Performance

Order of magnitude increase in write speed.



## **APPLICATIONS**



© Copyright 2009

## **Open Science**

- Supersonic inlet/isolator model
- Shockwave boundary layer interaction



- Conformal block boundaries
- Experimental comparison
- On-going work

DRESSER RAND



## Optimization

- D-R utilizes optimization techniques for enhancing turbomachinery design
- Results for perturbed database designs
- Analyze multi-dimensional data
- Database refinement **Optimization History** desigr var's launch Tolerance sensitivity >100,000 compute cores V2 ensemble Iteration Train meta-model Automatic Launch Decision: Process multiaeometry 8 optimization var's & ranges dimensional design / grid generation search database performance space data launch solution

Titan – An enabling technology for accelerating turbomachinery R&D.



#### Impact on Time-to-Solution





#### Summary

- Development efforts to enable scalable solver execution on OLCF hardware.
- The GPU acceleration of the solver module
  - The CPUBooster convergence acceleration module ported to GPU
  - Restructuring and instrumentation of the CPUBooster module with OpenACC directives has yielded a global iteration speedup of 1.2X-1.7X
  - With proper code restructuring, OpenACC allows easy GPU acceleration



## Summary

- The use of the CPUBooster module along with the Titan GPUs results in a 2.5X decrease in turnaround time and resource usage for D-R's optimization work.
- Large scale optimization related simulations are feasible due to availability of access to Titan
- Successful porting of the CPUBooster module has led to a new development program to port additional solver modules to execute on GPUs.



#### Acknowledgements

This research used resources of the Oak Ridge Leadership Computing Facility at the Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DEAC05-000R22725.

- Dr. Jack Wells, Director of Science, ORNL
- Suzy Tichenor, Director of Industrial Partnerships, ORNL
- David Gutzwiller and Mathieu Gontier, Numeca
- John Levesque (CRAY)
- Jeff Larkin (Nvidia)
- Dresser-Rand Employees











#### Questions

