National Combustion Code: Parallel Performance

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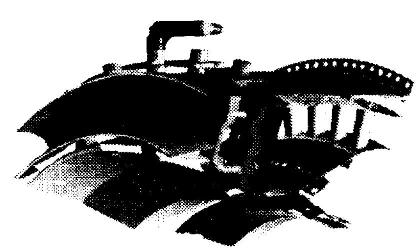
National Combustion Code (NCC)

- Code Description
  - Integrated system of codes for the design & analysis of combustion systems
  - Advanced features to meet designers' requirements for model accuracy and turn-around time
  - Industry/government development team
  - Primary flow solver is CORSAIR-CCD
- Fundamental Features at Inception
  - Unstructured mesh
  - Parallel processing



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NCC Performance Improvement Effort

- Achieve a 15-hour turnaround time with NCC on a large-scale, fully reacting combustor simulation by September 1998.
- The current goal is to achieve a 3-hour turnaround of a full combustor simulation (1.3 million elements) using CORSAIR-CCD by September 2001. This will represent a 1000:1 reduction in turnaround time relative to 1992.

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Benchmark Test Cases

- Lean direct-injection / multiple Venturi swirler (LDI-MVS) combustor
  - ~444,000 computational elements
  - Finite-rate chemistry (12 species, 10 steps)
  - All turbulence, species and enthalpy equations turned on
  - Estimated converge at 10K iterations
- The benchmark geometry to satisfy the NPSS milestones should be in the range of 1.3 million elements.
- A second LDI-MVS test case is also available with ~971,000 elements.

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Benchmark Hardware Platforms

Hardware Platform

- IBM SP-2
  - 144 RS6000/590s
- SGI Origin 2000
  - 64 & 256 250 MHz, R1000 processors

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Baseline Performance

- Test case
  - LDI-MVS combustor (444K elements)
  - Finite-rate chemistry (12 species, 10 steps)
  - Platform: IBM SP-2
- Performance
  - 64 processors
  - 61.4 secs/iteration
- Estimated convergence in 10,000 iterations for 171 hours.
- Estimated convergence for a 1.3 million element combustor is 512 hours.

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Significant Performance Improvements

- Algorithm modifications
- Code streamlining
- Deadlock elimination
- Hardware upgrades
- IDLM kinetics module
- SGI FORTRAN I/O library
- Domain decomposition strategy

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Algorithm Modifications

- CORSAIR-CCD uses a four-stage Runge-Kutta algorithm.
  - The convective, viscous and artificial dissipation terms were originally computed at each stage.
- The algorithm was modified:
  - The convective terms continue to be computed at each stage.
  - The viscous and artificial dissipation terms are computed at first stage and held constant for the remaining stages.
- This modification eliminated substantial computation and cut the required message passing in half.

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Performance Following Algorithm Modifications

- Test case
  - LDI-MVS combustor (444K elements)
  - Finite-rate chemistry (12 species, 10 steps)
  - Platform: IBM SP-2
- Performance
  - 84 processors
  - 28.5 secs/iteration
- Estimated convergence in 10,000 iterations or 79 hours.
- Estimated convergence for a 1.3 million element combustor is 238 hours.

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Performance Profiling Results: Code Streamlining

54% of time spent in two chemistry routines

- 40.1% chdiff (calculates viscosity and thermal conductivity of the gas mixture)
- 13.8% chprop (solves for gas-phase temperature and update gas-phase specific heat)
- 4.7% derivatives (calculate the 1st order derivatives)
- 4.4% chmsol (solves the linear systems of equation)
- 4.1% residual_smoothing
- 2.0% chmscc (calculates the coefficient matrix and B vector)

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Code Streamlining (continued)

- Streamlined finite-rate chemistry operations
  - Replaced "a**0.25" with "sqrt(sqrt(a))".
  - Eliminated unnecessary indexing of temporary variables.
  - Relocated some operations to an initialization routine.
  - Several divisions operations were replaced by their multiplicative inverse.

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Performance Following Code Streamlining

- Test case
  - LDI-MVS combustor (444K elements)
  - Finite-rate chemistry (12 species, 10 steps)
  - Platform: IBM SP-2
- Performance
  - 84 processors
  - 14.8 secs/iteration
- Estimated convergence in 10,000 iterations or 41 hours.
- Estimated convergence for a 1.3 million element combustor is 123 hours.

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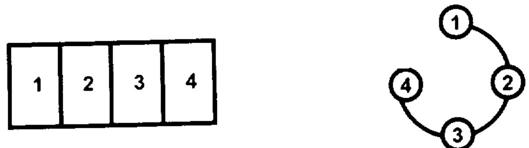
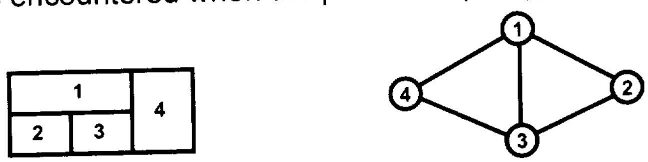
Deadlock Elimination

- The existing communication scheme was sufficient with a simple process topology.



- Deadlock was encountered when the process topology became more complex.



- A new communication scheme was developed to handle any arbitrary configuration of processes.
- This modification allowed increasing the number of processors used from 84 to 96.

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Performance Following Deadlock Elimination

- Test case
  - LDI-MVS combustor (444K elements)
  - Finite-rate chemistry (12 species, 10 steps)
  - Platform: IBM SP-2
- Performance
  - 96 processors
  - 13.0 secs/iteration
- Estimated convergence in 10,000 iterations or 36 hours.
- Estimated convergence for a 1.3 million element combustor is 108 hours.

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Hardware Upgrade

- IBM SP-2
  - 96 processors
  - 13.0 secs/iteration
  - Speedup = ~80.4
  - Efficiency = ~84%
- SGI Origin 2000
  - 32 processors
  - 10.1 secs/iteration
  - Speedup = 26.3
  - Efficiency = 82%

- A 1.3 x improvement in performance was realized by switching to the SGI Origin.
- Estimated convergence for a 1.3 million element combustor is 84 hours.

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Hardware Upgrade

- IBM SP-2
  - 32 processors
  - 34.4 secs/iteration
  - Speedup = ~30.4
  - Efficiency = ~95%
- SGI Origin 2000
  - 32 processors
  - 10.1 secs/iteration
  - Speedup = 26.3
  - Efficiency = 82%

- A 3.4 x improvement in performance was realized when comparing 32 processor results on the SGI Origin.

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ILDM Kinetics Module

- Intrinsic low-dimensional manifold (ILDM)
- Replaced the existing finite-rate chemistry module
  - Solve two scalar equations rather than 12 equations for species.
  - Species are obtained from the ILDM tables.
  - Properties such as density, viscosity, temperature can be obtained from ILDM tables.
  - Computation and message passing cost are reduced considerably.

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Performance with the ILDM Kinetics Module

- Test case
  - LDI-MVS combustor (444K elements)
  - ILDM Kinetics Module
  - Platform: SGI Origin 2000
- Performance
  - 32 processors
  - 2.1 secs/iteration
- Estimated convergence in 10,000 iterations or 6 hours.
- Estimated convergence for a 1.3 million element combustor is 18 hours.

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SGI FORTRAN I/O Library

- Scaling improved by switching to SGI f90 compiler.
  - Performance did not change when using <= 32 processors.
  - Performance improved when using > 32 processors.
  - Initialization time decreased dramatically.
- The SGI f90 I/O library handled multiple processes accessing the same file much more efficiently than the SGI f77 I/O library.
  - Each process was printing a residual to the standard output.

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Domain Decomposition Strategy

- METIS* grid partitioning tool (Univ. of Minnesota) was used to provide an alternative domain decomposition strategy for NCC.
  - The interface between processes is minimized.
  - Each process communicates with more of its neighbors, but the size of each message is much smaller.
- Code scalability is greatly improved on the Origin 2000, allowing an increase in the number of processors being used efficiently.

* Metis is a Greek word meaning 'wisdom.'

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Performance with the METIS Grid Partitioning Tool

- Test case
  - LDI-MVS combustor (444K elements)
  - ILDM kinetics module
  - Platform: SGI Origin 2000
- Performance
  - 96 processors
  - 0.69 secs/iteration
- Estimated convergence in 10,000 iterations or 1.9 hours.
- Estimated convergence for a 1.3 million element combustor is 5.8 hours.

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Performance with the METIS Grid Partitioning Tool

- Test case
  - LDI-MVS combustor (971K elements)
  - ILDM kinetics module
  - Platform: SGI Origin 2000
- Performance
  - 96 processors
  - 1.37 secs/iteration
- Estimated convergence in 10,000 iterations or 3.8 hours.
- Estimated convergence for a 1.3 million element combustor is 5.1 hours.

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National Combustor Code (NCC) Performance Timeline

- The current goal is to achieve a three-hour turnaround of a full combustor simulation (1.3 million elements) using CORSAIR-CCD by September 2001. This will represent a 1000:1 reduction in turnaround time relative to 1992.
- 1992: Estimated time to solution was 3,072 hours.
- 1995: Time to solution was 500 hours.
- 1999: Time to solution was 9 hours.
- 2000: Time to solution is 6 hours.
- Currently at 512:1 turnaround time.

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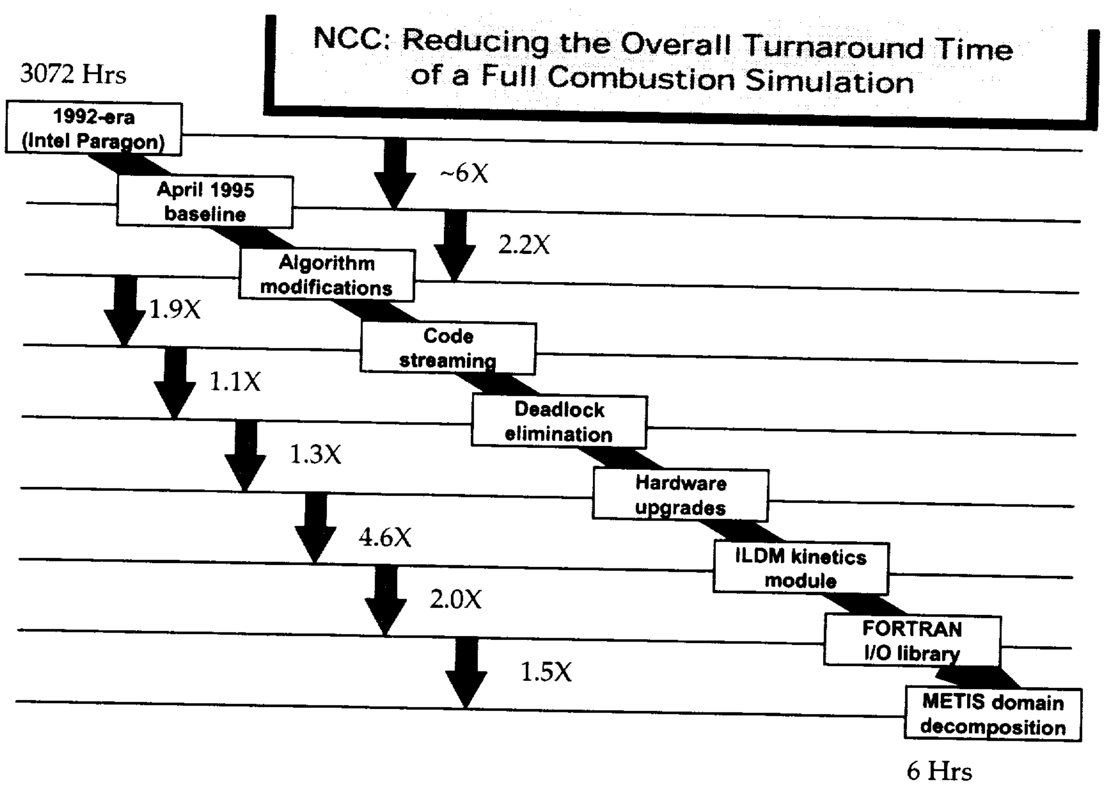

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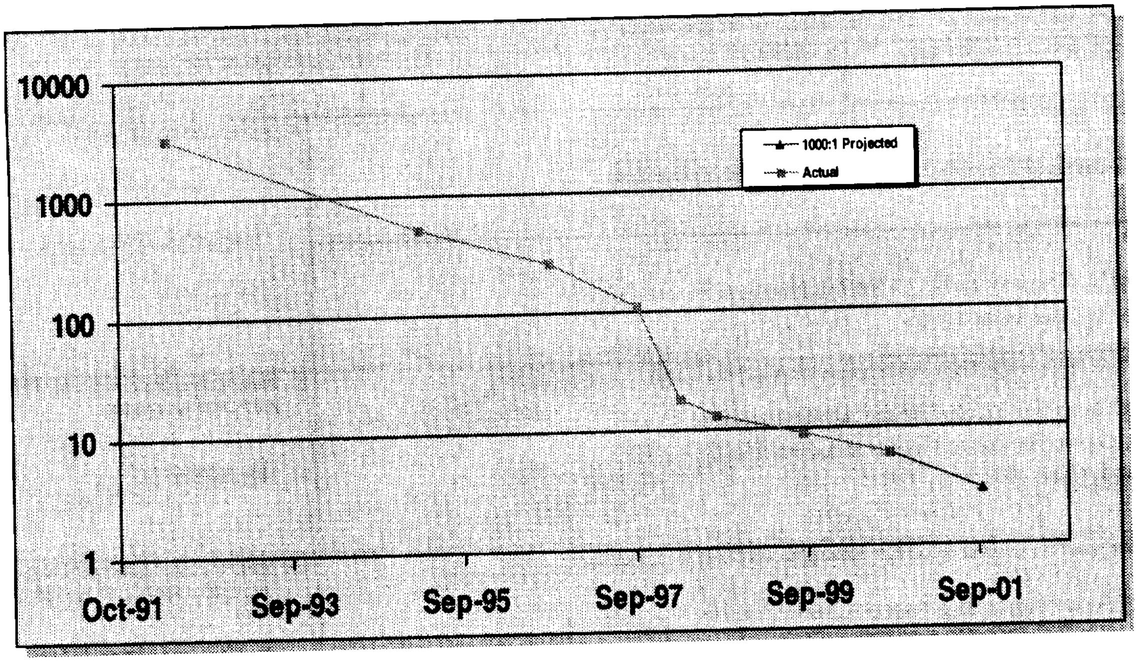
NCC: Estimated Reduced Turnaround Time



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Future Work Planned

- Investigate mixing message passing with shared memory programming to enable using additional processors more efficiently.
  - Continue to use MPI for existing domain-level, coarse-grained parallelism.
  - Investigate using OpenMP for loop-level parallelism.

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REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. AGENCY USE ONLY *(Leave blank)*

2. REPORT DATE
June 2001

3. REPORT TYPE AND DATES COVERED
Conference Publication

4. TITLE AND SUBTITLE
2000 Numerical Propulsion System Simulation Review

5. FUNDING NUMBERS
WU–725–10–11–00

6. AUTHOR(S)
John Lytle, Gregory Follen, Cynthia Naiman, Joseph Veres, Karl Owen, and Isaac Lopez

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
National Aeronautics and Space Administration
John H. Glenn Research Center at Lewis Field
Cleveland, Ohio 44135–3191

8. PERFORMING ORGANIZATION REPORT NUMBER
E–12452

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
National Aeronautics and Space Administration
Washington, DC 20546–0001

10. SPONSORING/MONITORING AGENCY REPORT NUMBER
NASA CP—2001-210673

11. SUPPLEMENTARY NOTES
Proceedings of a conference held at and sponsored by NASA Glenn Research Center, Cleveland, Ohio, October 4–5, 2000. Responsible person, John Lytle, organization code 2900, 216–433–3213.

12a. DISTRIBUTION/AVAILABILITY STATEMENT
Unclassified - Unlimited
Subject Category: 07 Distribution: Nonstandard
Available electronically at http://gltrs.grc.nasa.gov/GLTRS
This publication is available from the NASA Center for AeroSpace Information, 301–621–0390.

12b. DISTRIBUTION CODE

13. ABSTRACT ***(Maximum 200 words)***

The technologies necessary to enable detailed numerical simulations of complete propulsion systems are being developed at the NASA Glenn Research Center in cooperation with industry, academia and other government agencies. Large scale, detailed simulations will be of great value to the nation because they eliminate some of the costly testing required to develop and certify advanced propulsion systems. In addition, time and cost savings will be achieved by enabling design details to be evaluated early in the development process before a commitment is made to a specific design. This concept is called the Numerical Propulsion System Simulation (NPSS). NPSS consists of three main elements: (1) engineering models that enable multidisciplinary analysis of large subsystems and systems at various levels of detail, (2) a simulation environment that maximizes designer productivity, and (3) a cost-effective, high-performance computing platform. A fundamental requirement of the concept is that the simulations must be capable of overnight execution on easily accessible computing platforms. This will greatly facilitate the use of large-scale simulations in a design environment. This paper describes the current status of the NPSS with specific emphasis on the progress made over the past year on air breathing propulsion applications. Major accomplishments include the first formal release of the NPSS object-oriented architecture (NPSS Version 1) and the demonstration of a one order of magnitude reduction in computing cost-to-performance ratio using a cluster of personal computers. The paper also describes the future NPSS milestones, which include the simulation of space transportation propulsion systems in response to increased emphasis on safe, low cost access to space within NASA's Aerospace Technology Enterprise. In addition, the paper contains a summary of the feedback received from industry partners on the fiscal year 1999 effort and the actions taken over the past year to respond to that feedback. NPSS was supported in fiscal year 2000 by the High Performance Computing and Communications Program.

14. SUBJECT TERMS
Engine design; Gas turbines; Rocket engines; Computerized simulation

15. NUMBER OF PAGES
111

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
Unclassified	Unclassified	Unclassified	