PARALLEL COMPUTATION IN NGPDL

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May 2014

BACKGROUND

- Many NGPDL members are using parallel/multi-core computers
- Available parallel resources:
  - National facilities (NASA, DOE, DOD, etc.): often requires competitive proposals to be written (requires Prof. Boyd's time!)
  - Local facilities (Flux): requires Prof. Boyd's funds!
  - Some members have multi-core desktop machines
- There is a temptation to keep increasing the number of processors in a run to decrease turn-around time
- **Question**: before investing in further local resources, are we making efficient use of our current resources?
- Today's meeting:
  - Hicham to discuss recent experience with LeMANS
  - Prof. Boyd to discuss recent experience with MPIC

HISTORY

- Wide range of codes/problems being worked on in NGPDL, giving a wide range of problem size and code performance:

Who	Where	Code	#-Cores	#Cells/Particles	Time	Efficiency	time/c-p/dt
Nick	nyx	LeMANS-**MHD**	32	2M-c	96 hrs	70-85%	100-500 μs
"	bighouse	"	30	3M-c	72 hrs	80-90%	50-400 μs
Erin	nyx	MONACO-PIC-1D	20	300k-p	180 hrs	50-80%	1.0 μs
Tyler	falcon (DoD)	MONACO-PIC-2D	16	300k-p	12 hrs	60-70%	
Alex	nyx	LeMANS-MOPAR	8	20k-c	8 hrs	65-75%	3,000 μs
Jon, Eunji	nyx	MONACO-LD	16	13M-p	32 hrs	60-80%	1.0 μs
Tim-D	pleiades (NASA)	MONACO	112	110M-p	100 hrs	70%	0.5 μs
"	"	MPC	8	30M-p	720 hrs	70-80%	0.5μs/100μs
Hicham	rtjones (NASA)	LeMANS	120	2M-c	48 hrs	60-80%	576 μs
Anna	nyx	LeMANS	8	20k-c	32 hrs	75-90%	310 μs
T. White		DPLR (2D, 1-species)	10				15-150 μs

Parallel performance of NGPDL codes as of 01-18-2010

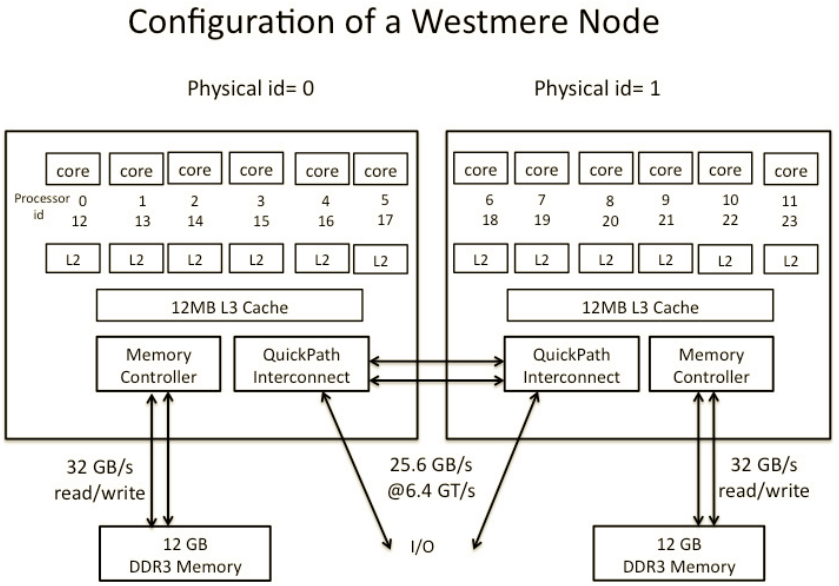
*LeMANS-**MHD** is running with full chemistry and the coupled MHD module (requires 100-10k sub-steps) to converge per iteration.

PLEIADES SUPERCOMPUTER

LeMANS Parallel Efficiency Study on Pleiades Supercomputer

PLEIADES SUPERCOMPUTER

- 7th fastest supercomputer on the TOP500 list
- Includes 4,608 Intel Xeon X5670 (Westmere) nodes
  - 2 six-core processors per node (12 cores per node)
  - Processor speed: 2.93 GHz
  - 2 GB per core, 24 GB per node
  - Nodes connected with an InfiniBand interconnect (32 Gb/s)

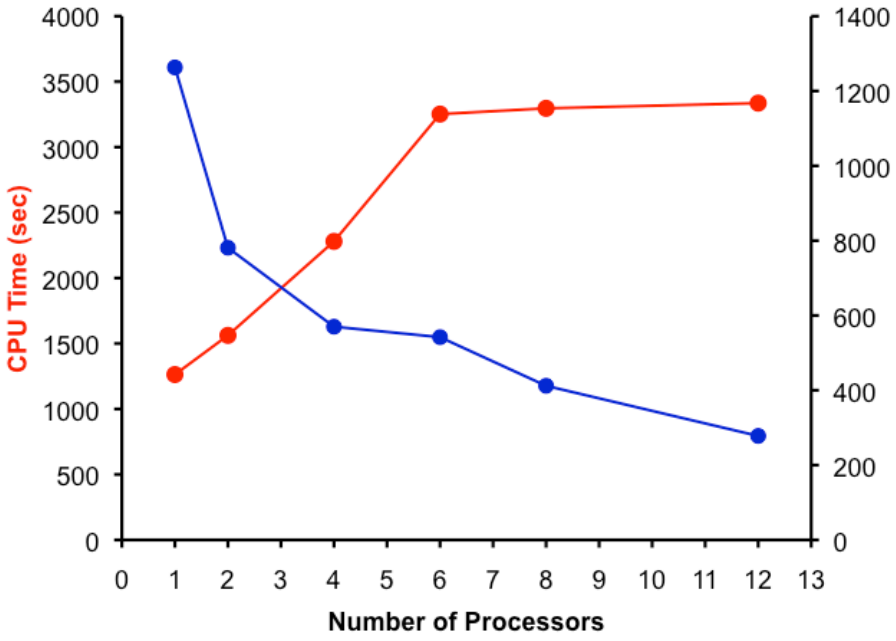


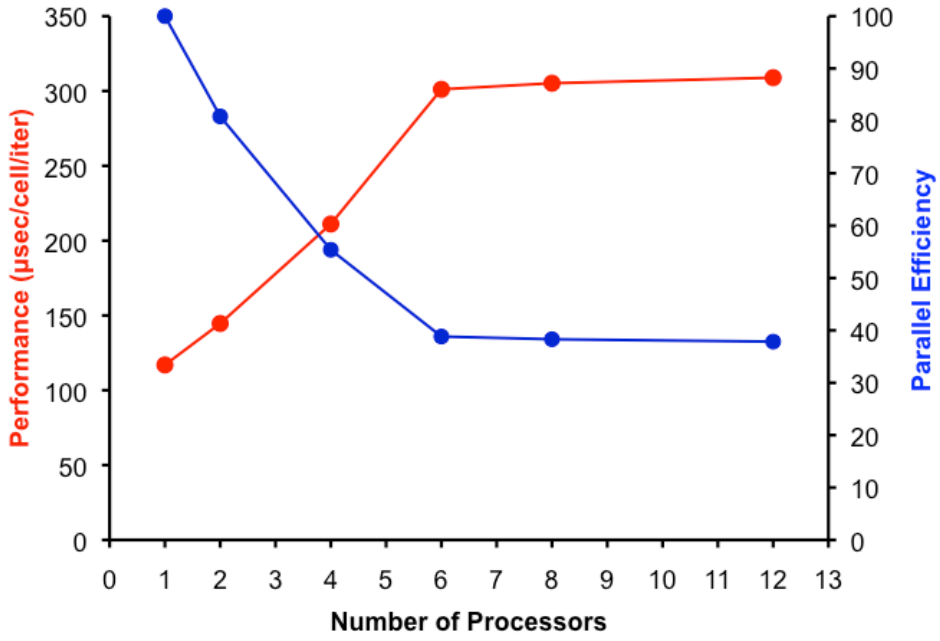
CASES

- Case 1:
  - 3D
  - Grid size: 60 x 60 x 60
  - Line-implicit time integration
  - 50 iterations with minimum I/O
  - Perfect gas (5 equations)
- Case 2:
  - 3D
  - Grid size: 60 x 60 x 60
  - Line-implicit time integration
  - 50 iterations with minimum I/O
  - 11 species with chemistry
  - Vibrational nonequilibrium (16 equations)

CASE 1
PERFECT GAS

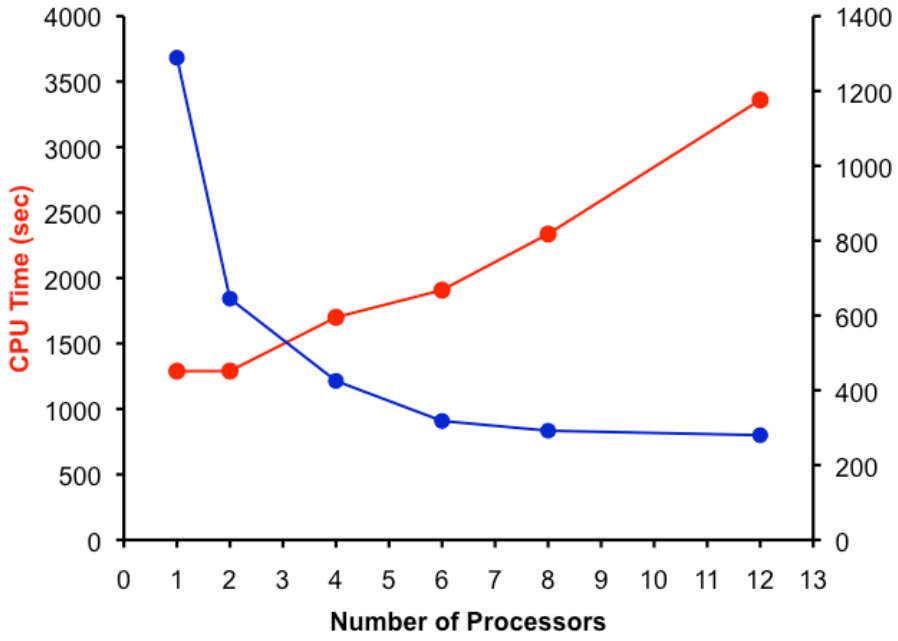
- Intel 10.1.021 C compiler with MPT 1.25 MPI Package
- 1-12 cores using only 1 node
- No appropriate process pinning

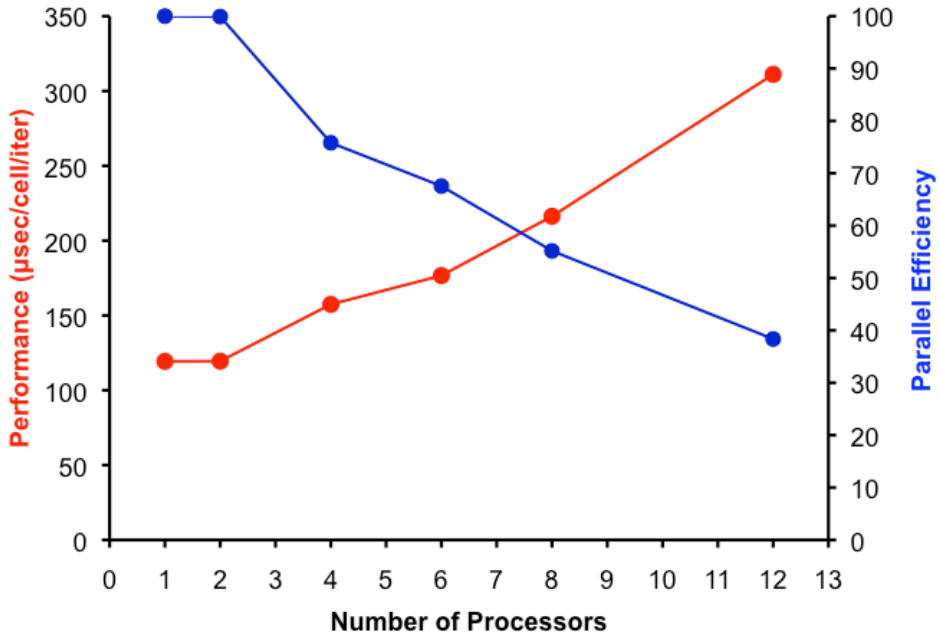




CASE 1
PERFECT GAS

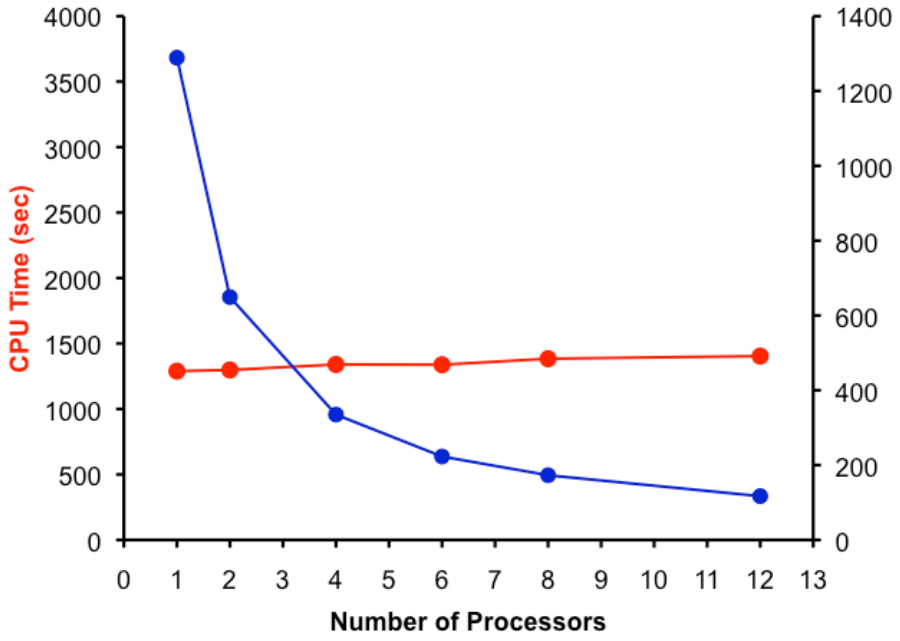
- *Intel 11.1.072 C compiler with MPT 2.04 MPI Package*
- 1-12 cores using only 1 node
- *Processes pinned to reduce memory bandwidth contention*

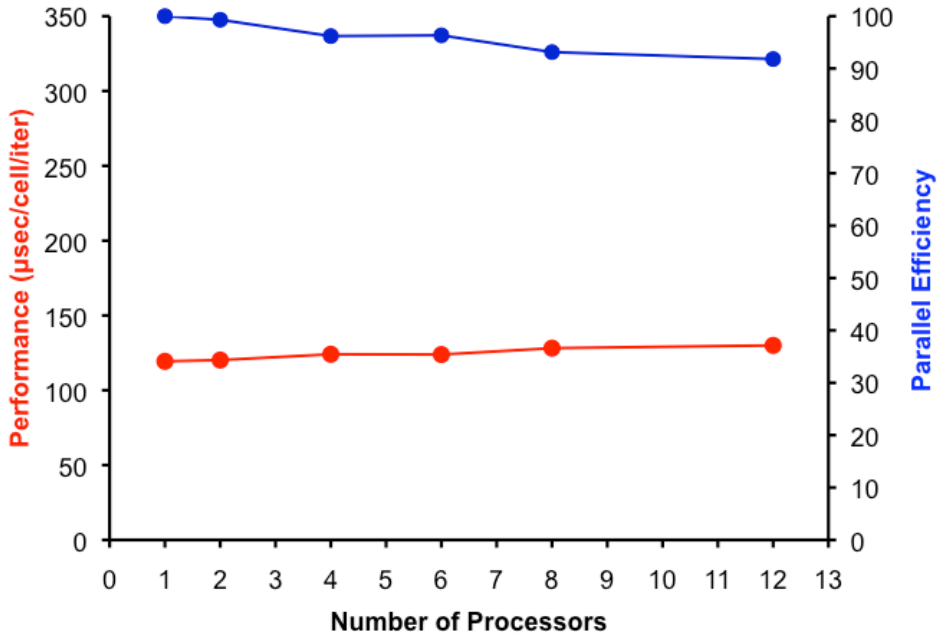




CASE 1
PERFECT GAS

- Intel 11.1.072 C compiler with MPT 2.04 MPI Package
- *1-12 nodes (1 core per node)*
- *Maximum memory access bandwidth*





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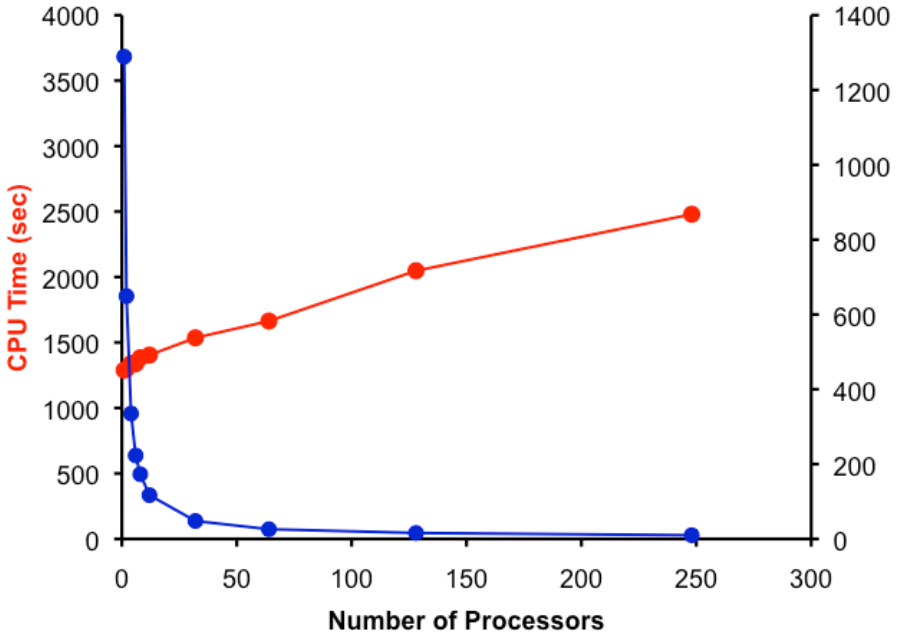
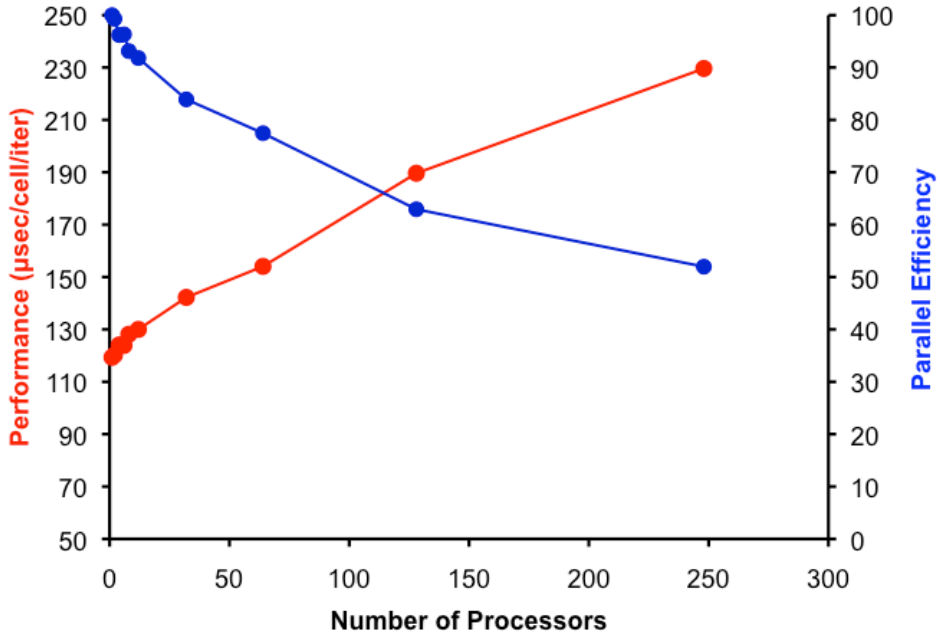
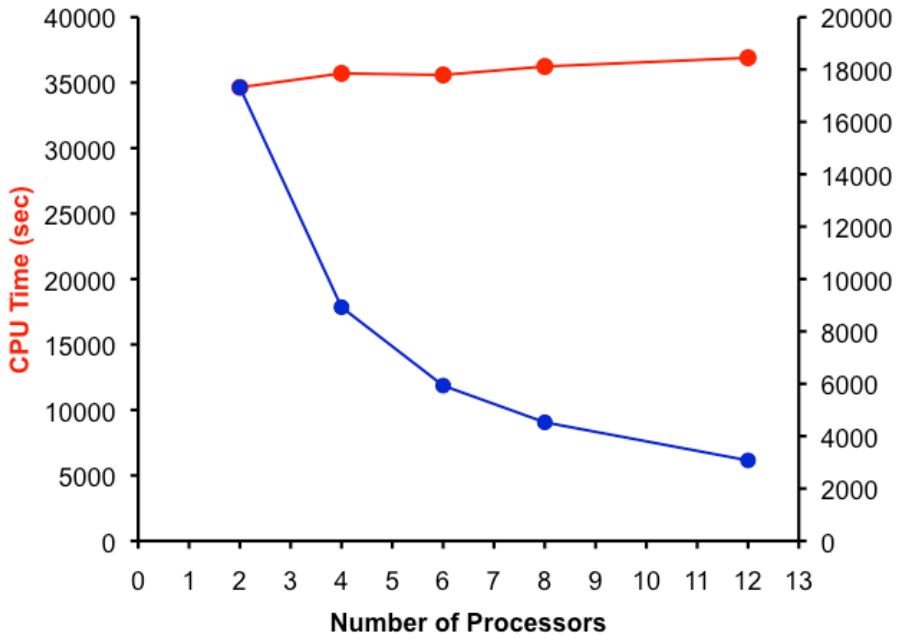
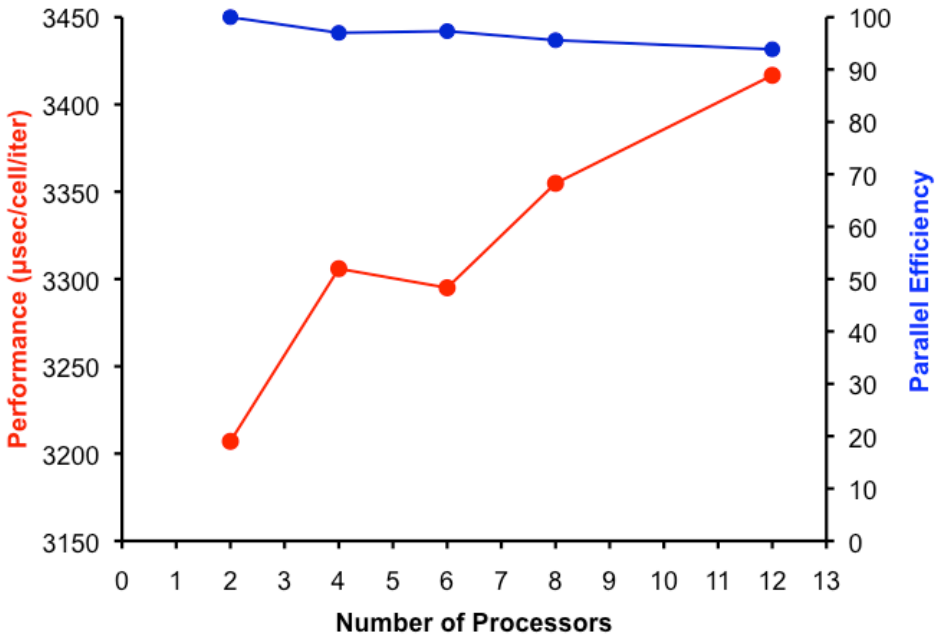




CASE 2
11 SPECIES, CHEMISTRY, VIBRATIONAL NONEQUILIBRIUM

- Intel 11.1.072 C compiler with MPT 2.04 MPI Package
- 2-12 cores using only 1 node
- Processes pinned to reduce memory bandwidth contention





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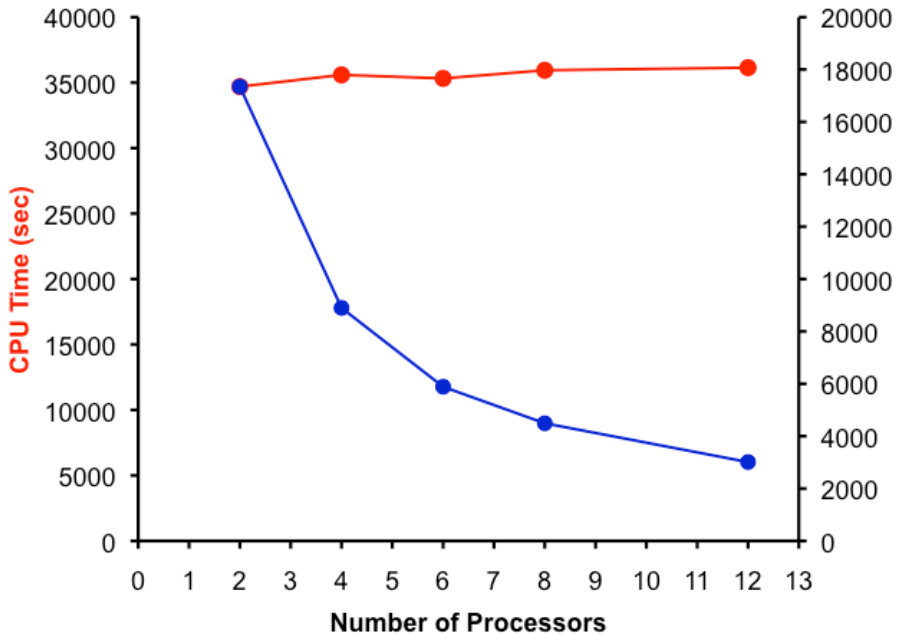

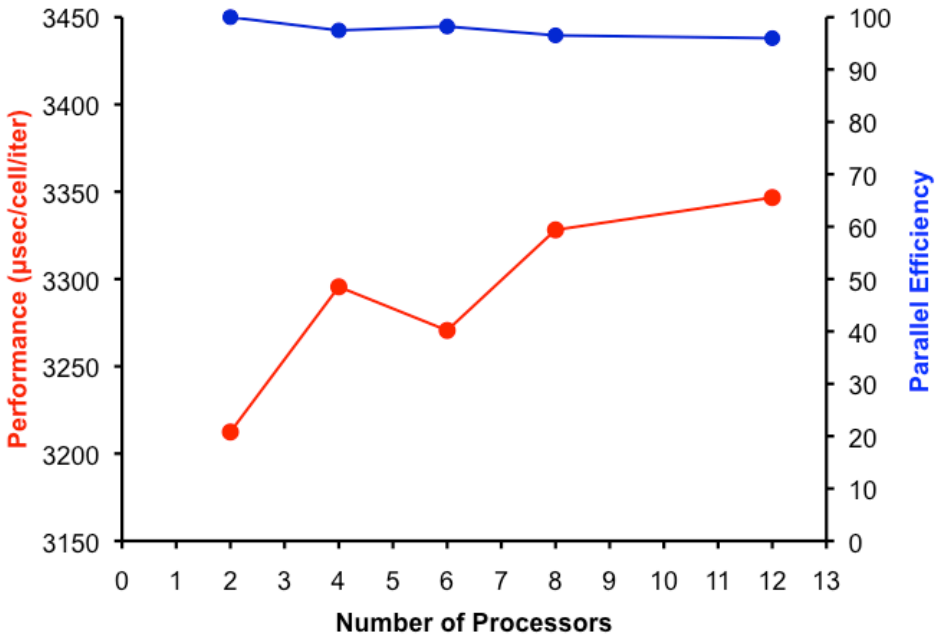

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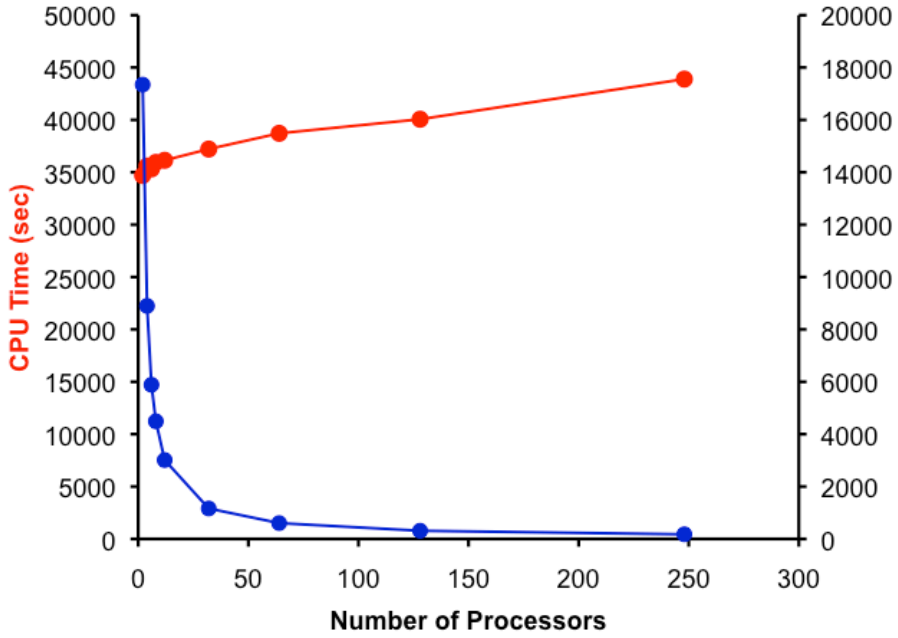

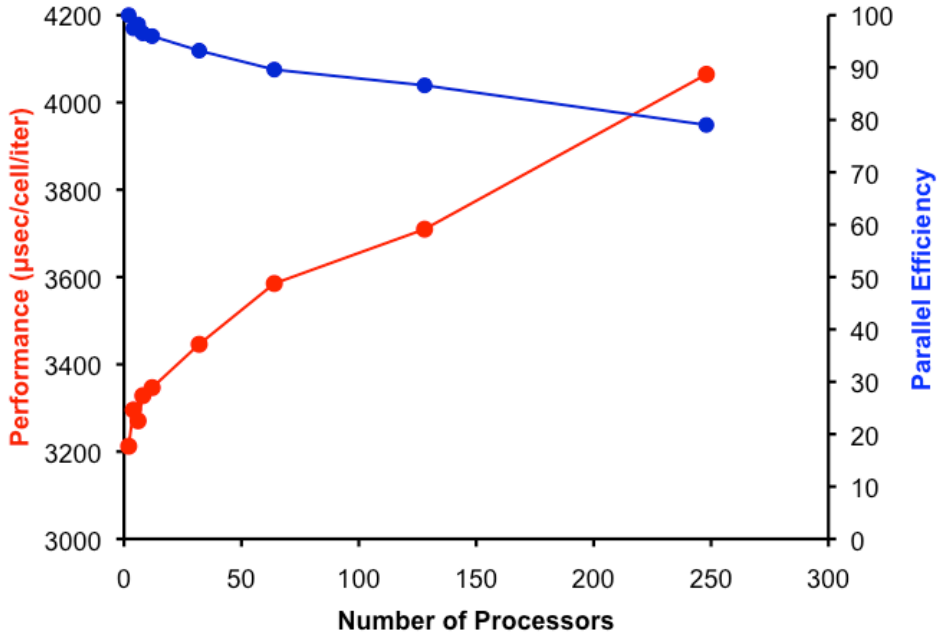

COMPARISON WITH OTHER CFD CODES
US3D

- US3D – CFD code for simulating hypersonic, reacting flows developed at University of Minnesota
- Results obtained on dual-processor, dual-core, 2.2 GHz, AMD Opteron nodes with 4 GB of memory per node
- Nodes connected with a Myrinet interconnect (2 Gb/s)
- 3D, 50 x 50 x 50 grid, 100 iterations, line-implicit time integration method
- Both perfect gas (5 equations) and 11 species air chemistry (16 equations) simulations

I. Nompelis, T. Wan, and G. V. Candler, "Performance Comparisons of Parallel Implicit Solvers for Hypersonic Flow Computations on Unstructured Meshes," AIAA Paper 2007-4334, June 2007.

COMPARISON WITH OTHER CFD CODES
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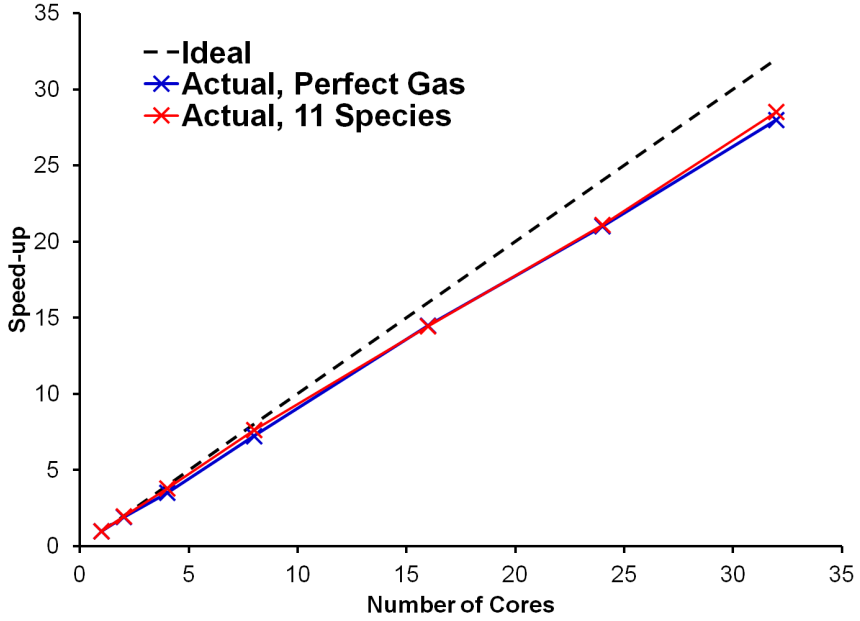
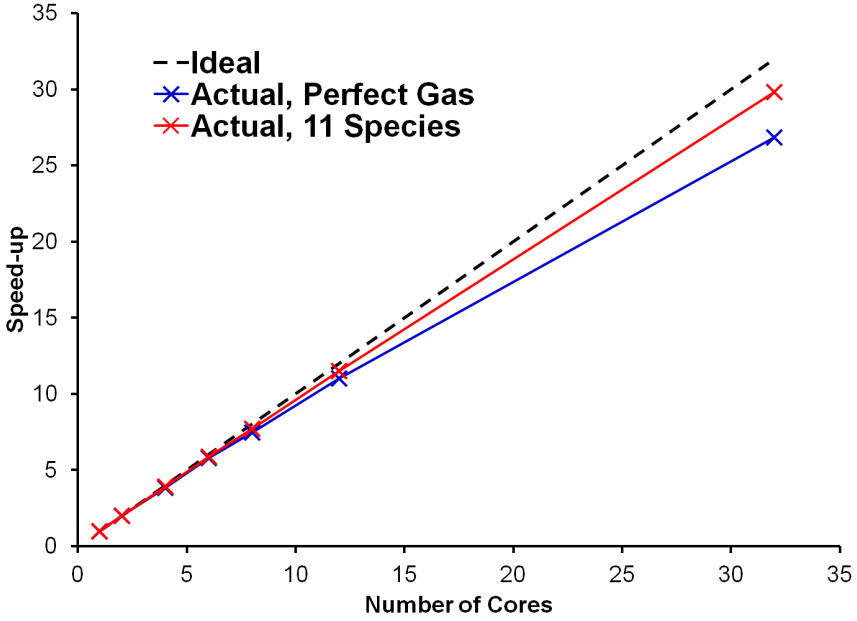


LeMANS



MONACO-PIC Parallel Efficiency Study on NYX Supercomputer

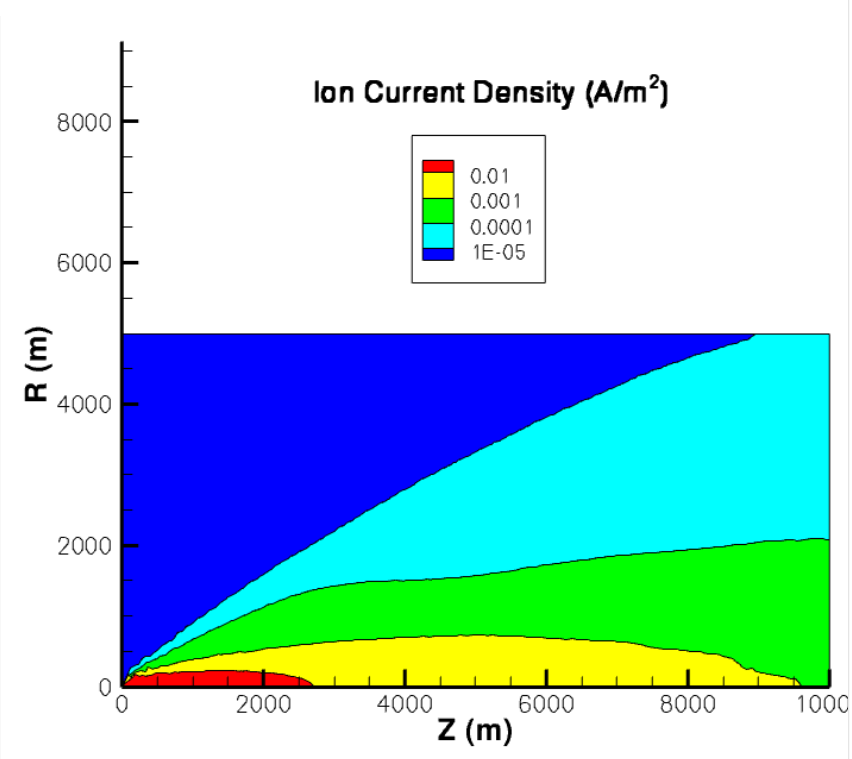
MONACO-PIC TEST CASE

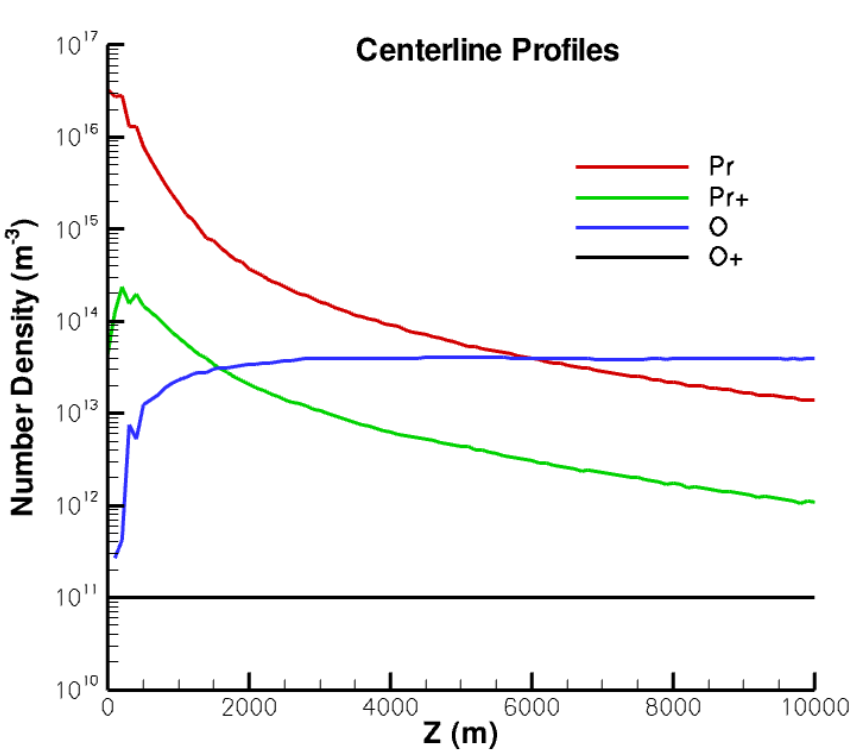
- MPIC simulation of rocket plume interacting with atmosphere

- Assumptions and conditions:
  - Space Shuttle thruster firing at MFR=0.2 kg/s
  - 450 km altitude (V=8 km/s; O: 4×10^{13} m^{-3}; O+: 10^{11} m^{-3})
  - Single propellant species (Pr)
  - Ion (Pr+) formed through CEX with atmospheric O+

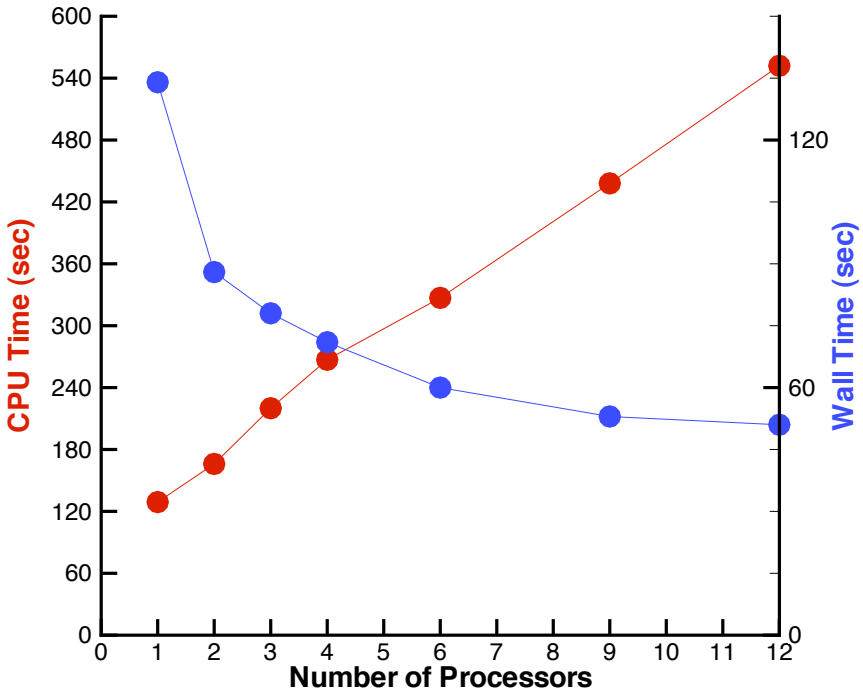
- Numerical details:
  - Flow domain of 10 km x 5 km
  - DSMC+PIC
  - 1.8 million particles, 12 processors, 3 hours CPU time

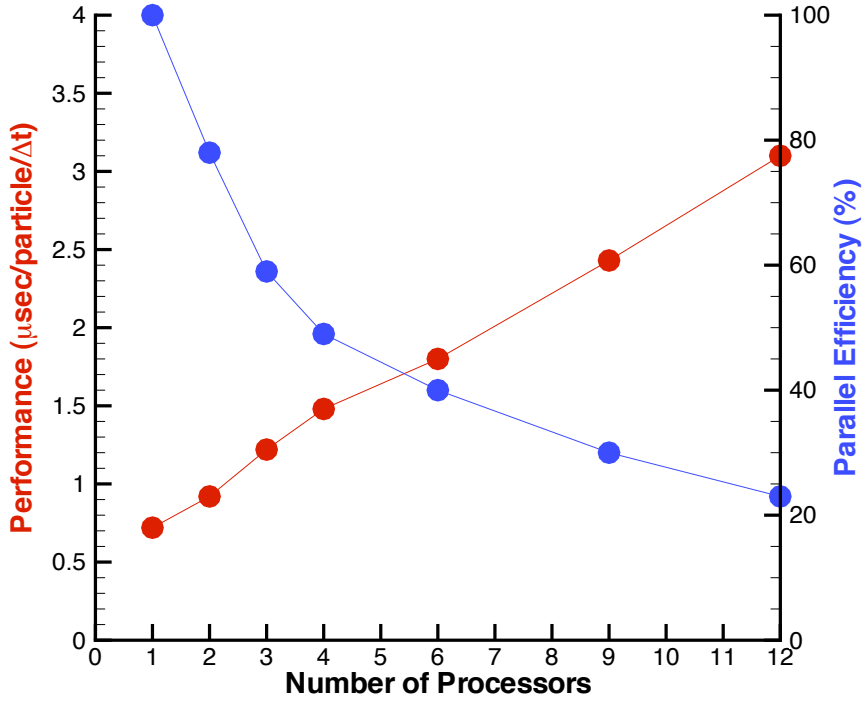
FLOW FIELD RESULTS





CODE PERFORMANCE (100 ITERATIONS)





CONCLUSIONS

- We should aim for and expect to be able to run ALL parallel computations at some minimum parallel efficiency (e.g. 70%)
- It is unacceptable scientifically and unfair to other system users to run below that efficiency
- There is a need to search for the “sweet spot” of operation of your code on your computer system:
    - LeMANS: depends mainly on #-cells / processor
    - MONACO: depends mainly on #-particles / processor, and in some cases #-collisions may also be important
- Parallel code performance is a moving target:
    - The source codes are constantly changing
    - Compilers and hardware change periodically