Scientific Computing: Where Does MPP Fit in?

Timothy J. Williams

National Energy Research Supercomputer Center

Overview

- Characterization of computational science
- Computer species
- Who needs MPP now?
- Who does MPP now?

Character of Scientific Computation

- Algorithms evolve, sometimes with physics.
  - Often not “canned” algorithms
- Large blocks of floating-point arithmetic.
- Testing on a new platform may be *highly* non-trivial.
  - Different machine arithmetic, non-identical answers
  - Physics codes can run happily with bugs
    - May require several long, expensive physics runs to notice the bug; more to figure it out.
      - Debuggers don’t allow saving state
    - Small test-case runs may be useless for debugging
      - Small enough for 1 MPP node may be physically absurd.

Character of Scientific Programmers

- Prefer a high-level approach to programming
  - The language they know, unless you have *proof* that something else is better
  - No assembly coding
  - Same code on all platforms
  - Opinions of the formal computer science community regarded skeptically
  - Exceptions to the above may be made for something fun
    - Parallel programming is rarely fun
- Usually grounded in numerical analysis
  - Academic education in numerical analysis is shared-memory serial

Computer Species for Scientific Programming

- Superscalar workstation: not quite big and fast enough for all
- Cluster of workstations (COW): too expensive to scale up to MPP size
- Shared-memory parallel vector processor (PVP) [C90]: Great!
  - Static RAM means even gather/scatter operations are fast
  - Fairly large memory
  - Excellent optimizing compilers
    - Ten years development of good vectorizing compilers after introduction of first Cray
  - Just keep making them bigger and faster! (And cheaper!)
- Symmetric Multiprocessor (SMP) with superscalar CPUs: ???
  - Dynamic RAM means gather/scatter operations are slow
  - Fairly large memory
  - Starting on ten years of development of good caching compilers
- Distributed-memory massively parallel processor (MPP): "You must love it." [Apologies to George Orwell]
  - Really large memory
  - Starting now on developing *any* parallel compilers (HPF)
- Hierarchical machines (SMPs + fast network):??????

Can One Program Run Well on All Species?

- Fortran 77 program: no
  C program: no
  C++ program: no
  <insert serial programming language here> program: no

NERSC MPP Workshop will point out techniques for portability using various parallel programming paradigms

- Message passing
  - Collapse to serial code on one node
  - Portability already demonstrated
- High Performance Fortran (HPF)
  - Collapses to Fortran 90 on one node
    - F90 is the way of the future (certainly for Fortran)
- Special parallel languages (PCP, Sisal, Mentat,....)
  - Collapse to serial code on one node
- High-level methods, like object-oriented
  - Hidden parallel abstraction layers can include serial
- In general: MPP parallelism implies good parallelism on SMP (but *not* vice-versa)

Overcoming Fear Wasted Effort on MPP

- Worst-case scenario: MPP market collapses
  - Working on parallel programming reveals concurrency
    - Helps on PVP and SMP architectures
  - Working on MPP's with cache+superscalar nodes reveals caching strategies
    - Helps on workstation and SMP architectures
- Unpleasant scenario: My favorite MPP manufacturer collapses
  - Portable methods will port to survivor machines
    - If manufacturers ignore demands to support portable programming systems (MPI, HPF), they deserve to die.
  - Nonportable methods will not port to survivor machines
    - If the scientist-programmer "throws his body at the machine"[1] to program it, he gets hurt twice:
      - bouncing off
      - hitting the ground

1. P. Dubois (paraphrased)

Who Needs MPP *Now*?

- Those needing *scalability* to large numbers of processors for:
  - Memory size (MPP memory size scales with #processors)
    - SMP, PVP, and scalar workstation memory sizes technologically limited
      - Unless you have scalable dollars to pay (maybe)
    - For local (on-node) memory references, MPP aggregate memory access bandwidth scales with #procs
  - Compute speed (MPP compute speed scales with #procs)
    - Modern MPP processor interconnection networks scale up in aggregate bandwidth with #procs
      - ⇒ Communication in scalable parallel programs not a bottleneck to compute speed scaling with #procs
- Grand Challenge problems, including those not deemed as such by HPCC

Character of Programs Needing MPP

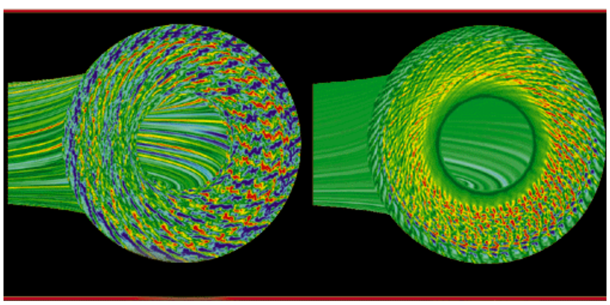
- 3D
  - Lots-o-memory
- Modelling phenomena with disparate spatial scales
  - Lots of grid points (uniform or nonuniform mesh)
- Turbulence modelling
  - You can never have high enough Reynold’s number
- Very basic physics models
  - Lattice quantum chromodynamics (QCD)
    - 4D
  - Plasma particle-in-cell (PIC)
  - Molecular dynamics
  - N-body problems
    - You can never have enough bodies
- Large simulation domain
  - Global climate modelling

Current MPP Scientific Computing Projects

- Limited survey of current work on using MPP in real computational science projects.
- Related to NERSC interests, if not actual NERSC projects.
- Names listed are not necessarily project leaders or contacts
  - Many projects are multi-institutional
- If any of these are related to your project, you should see what they’ve done before you proceed.
- List some WWW pages, reports, papers.
  - WWW pages often have links to online preprints/reports.

Gyrofluid Plasma Simulation

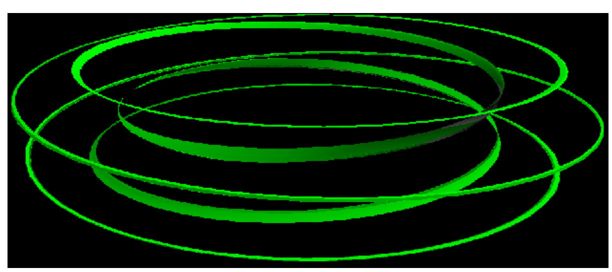
- Solve fluid moments of gyrokinetic equation
  - Simulates tokamak core turbulence & cross-field transport



  - http://www.nersc.gov/doc/Comp_Research/Comp_Physics/tokamak.html
- Gary Kerbel (NERSC), *et.al.*
  - Phase 2 talk at MPP Workshop
- Data parallel (CM Fortran)
- Numerical Tokamak Project (HPCC)

Gyrokinetic PIC Simulation

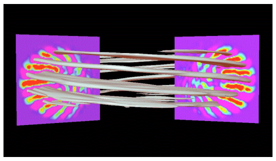
- Particle-in-cell simulation of gyrokinetic equation
  - Simulates tokamak core turbulence & cross-field transport
- Tim Williams (NERSC), Andris Dimits (LLNL)
  - Phase 2 talk at MPP Workshop
  - Slab-geometry message-passing code developed
  - Toroidal flux-tube geometry message-passing code in debugging phase
    - Same physics as production code on C90 (SPP)

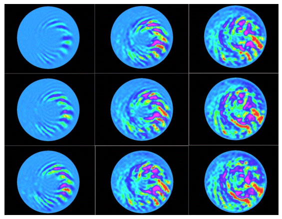


  - http://www.acl.lanl.gov/GrandChal/Tok/LLNLGyrokinetic/LLNLGyrokinetic.html
- Numerical Tokamak Project (HPCC)

Gyrokinetic PIC Simulation (cont'd)

- Scott Parker (PPPL), *et. al.*
  - Global toroidal geometry





  - Multitasking (C90-SPP), data-parallel (CM5)
    - Message-passing (T3D)--done/nearly done
  - http://www.nersc.gov/doc/buffer/may95/Cummings.html
  - Numerical Tokamak Project (HPCC)

Plasma Turbulence Simulation

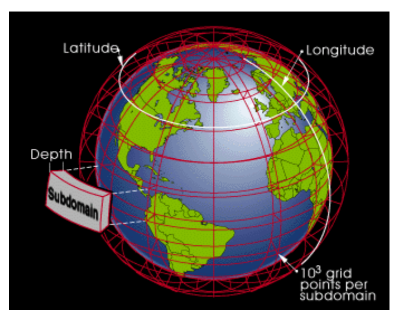
- DTEM fusion plasma turbulence simulation
  - Single fluid model appropriate for drift waves
  - 3D slab geometry (hooks in for toroidal effects)
  - Spectral in poloidal & toroidal angles
  - Finite difference in redial
  - J.N.Lebouef (ORNL), Tim Pierce(NERSC)
    - Phase 2 talk at MPP Workshop
  - Message-passing (PVM)
  - Hand-coded kernels for T3D

Computational Chemistry

- NWChem computational chemistry codes
  - Rick Kendall, *et. al.* (PNL)
    - Phase 1 talk at MPP Workshop
  - Programmed using Global Array Toolkit
    - Message-passing on MPP
    - Shared memory on SMP

Global Climate Modelling

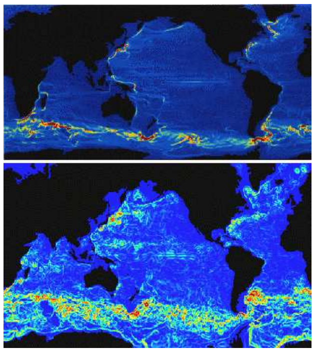
- CAMILLE and related codes
  - Art Mirin (NERSC), *et. al.*
  - Message-passing
    - Paragon, CM5, T3D, BBN,....



  - http://www.nersc.gov/doc/Comp_Research/Comp_Physics/climate.html

Global Climate Modelling (cont'd)

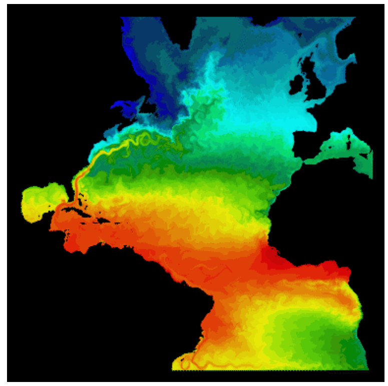
- Parallel Ocean Program (POP)



  - ❍ Bryan-Cox-Semtner ocean model
  - ❍ C90, CM5 (data-parallel), now T3D, Paragon
- Robert C. Malone, Richard D. Smith *et.al.* (LANL)
  - ❍ http:/http://www.acl.lanl.gov/HPCC/climate_1.html
- HPCC,CHAMMP

Global Climate Modelling (cont'd)

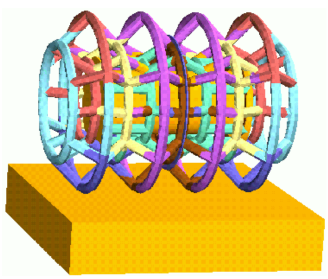
- Miami Isopycnic Coordinate Ocean Model (MICOM)
  - ❍ Matt O'Keefe, Aaron Sawdey (U. Minnesota); Rainer Bleck (U. Miami)
  - ❍ T3D (shmem library); SGI SMP (T3D emulation library)
    - ■ High-level layer above shmem for ports to other MPP
  - ❍ Atlantic basin simulation, 1437x1437 (0.08 degree); sea temperature



    - ■ 11 isopycnic (constant-density) layers
  - ❍ http://www-mount.ee.umn.edu/~sawdey/micom.html

Structural Mechanics

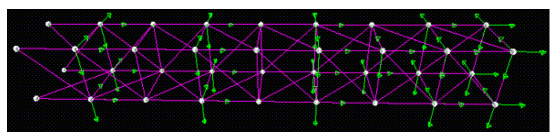
- DYNA3D finite-element code



  - ❍ Carol Hoover, *et.al.* (NERSC)
    - ■ Phase 2 talk at MPP Workshop
  - ❍ Meiko CS-2, Cray T3D

Structural Mechanics (cont'd)

- MAS: Massively Actuated and Sensed structures
  - ❍ Micro sensors and actuators positioned in structure
  - ❍ Model structural mechanics coupled with sensor/actuator feedback loop
  - ❍ Design adaptive structures



(note: "up" is "right" in this image)

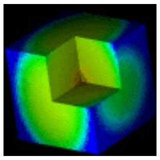
  - ❍ Goal: real-time simulation.
  - ❍ Ramesh Menon (U.Colorado), *et.al.*
  - ❍ http://caswww.colorado.edu/~rgmenon/project.html

Lattice Quantum Chromodynamics (QCD)

- MILC (MIMD Lattice Computation) Collaboration
- Multi-institutional HPCC Grand Challenge Application Group
- Claude Bernard (Wash. U), *et.al.*
- Message-passing, with high-level interface layer for scientist-programmers
  - Public domain source code
  - Widely portable (Intel Paragon, CM5, T3D)
    - Optimized assembly kernels
  - Production code
  - Paper: “Recent Progress on Lattice QCD with MIMD Parallel Computers,”
    http://physics.indiana.edu:80/~sg/milc/talk.ps
- NERSC user A.Soni now getting help/collaboration

Lattice QCD (cont’d)

- Rajan Gupta (LANL), *et.al.*



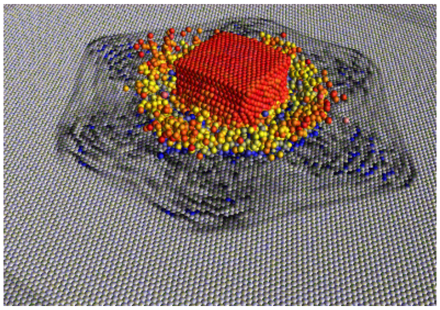
  - CM5: CM Fortran data-parallel (50000 lines) + CDPEAC kernels
    - 10 man-months to develop production code
    - Comparable performance per node with message-passing (MILC)
  - Conference paper: “Prospects of Solving Grand Challenge Problems”
    - Interesting points about machine architecture (memory access)
- http://nqcd.lanl.gov/Lattice_QCD/bluebook/Status_report1.html

Classical Molecular Dynamics

- Ames Laboratory classical molecular dynamics calculations
  - Embedded atom method
  - Direct modelling of solid-state phenomena
  - http://www.public.iastate.edu/~cmpthy/#MainAreasOfResearch
- Full production code on Paragon, nCube
  - Message-passing
  - Capable of 10^7 atoms on 512 node Paragon
- HPCC Materials Science Grand Challenge

Classical Molecular Dynamics (cont’d)

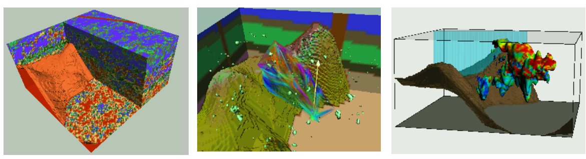
- SPaSM code



- Message-passing
  - Multi-cell approach
  - Up to 10^8 atoms on CM5
  - Force kernel coded in CDPEAC (60 lines)
- Peter Lomdahl (LANL)
- http://www.acl.lanl.gov/Lomdahl/spasm_intro.html

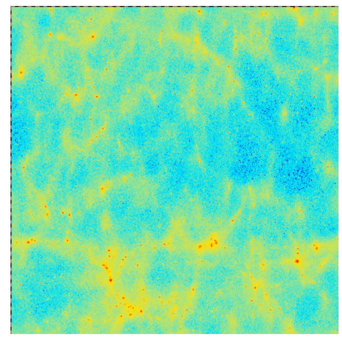
Porous Flow

- ParFlow
  - ❍ Subsurface groundwater flow modelling
    - ■ Multigrid-preconditioned conjugate gradient
      - ❑ Godunov approach in progress
    - ■ Message-passing (T3D, CM5, Paragon, nCube, Meiko CS2, workstations)
  - ❍ Chemical contaminant migration in groundwater
    - ■ Particle-in-cell method (C90; message-passing MPP project beginning)
  - ❍ Steve Ashby (LLNL), *et.al.*
  - ❍ http://www.nersc.gov:80/doc/Comp_Research/CCSE/ParFlow/
  - ❍ Heterogeneous conductivity field



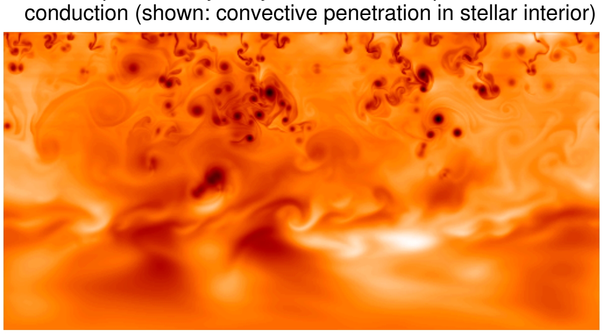
N-Body Cosmology

- GC^3 Grand Challenge Cosmology Consortium
- TPM parallel N-body program
  - ❍ Tree-based direct algorithm for high-density regions
  - ❍ Particle-mesh algorithm for low-density regions
  - ❍ Guohong Xu (Princeton)
  - ❍ http://zeus.ncsa.uiuc.edu:8080/TPM_simulation.html
  - ❍ Message-passing (PVM, MPL)
    - ■ Task (control) parallelism for tree calculation managed by master PE that computes global tree for a timestep
    - ■ COW, IBM SP2 machines



Astrophysical Turbulence

- 2D Compressible hydrodynamics with T-dependent thermal conduction (shown: convective penetration in stellar interior)



  - ❍ High-order Godunov method, multigrid elliptic solve
  - ❍ Message passing (IBM SP2, Intel Delta)
  - ❍ Robert Rosner, Fausto Cattaneo, Andrea Malagoli (U.Chicago).

EM Fields in Superconductors

- Time-dependent Ginzburg-Landau equations
  - ❍ BlockComm library (part of PETSc high-level interface for message-passing): IBM SP2
  - ❍ Rectangular block of superconductor embedded in block of normal conductor
  - ❍ Hans G. Kaper (ANL), *et.al.*
  - ❍ Penetration of magnetic field as quantized fluxoids (like vortices in fluid) into black superconducting zone