High Performance FORTRAN
Motivating Applications and User Feedback

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Also available as SCCS-692 from the Northeast Parallel Architectures Center at Syracuse University.
University of Maryland
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and
Syracuse University
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User Feedback
HPF Motivating Applications and
HPF Meeting (NPAC Technical Report SC7 692)
Overview:

- User Feedback
- Source Code Collection and Documentation
- Education and Training Material

Features:

• FTP/WWW sites at Maryland and Syracuse

(Syracuse)

- High Performance Fortran Applications (HPFA) project
- HPF-2 Motivating Applications collection effort (Maryland)
High Performance Fortran Applications 3

- Reviewing and editing existing material
- Other explanatory and training material

- Existing codes or new ones written to illustrate

- Need volunteers for:

  (>) >25 lines
  and long enough to illustrate something interesting
  Good = short enough to understand (>1000 lines)

  
  To provide good example codes.

  Premise: The best way to accelerate usage of HPF is

  Education, Training and Outreach
complicated for non-experts

Full Application: true test, may be too

Applications

Similar algorithms and tradeoffs to Full

Mini-Applications: simplified programs with

some feature or idiom

Kernels: fragments demonstrating use of

Application Categories
Motivating Applications Overview

- Clearly the choices of what to support with HPF-2
- Programming idioms representative of full-size codes
  - Computationally demanding problem domains
- Collect representative mini-applications
- If so, where are they going?
- Are programmers learning HPF behind?
- Goal: guide the extension or non-extension of HPF
High Performance Fortran Applications

- Required primitives not well understood
- e.g., Barnes-Hut tree for long-range N-body problems
  - Dynamic linked structures
  - Scalable I/O: out-of-core arrays; checkpointing.
  - Task parallel codes: CMU FX project examples of non-scalable subproblems.
- Irregular mapping and data motion as generalized reduction
  - Vortices, direct-simulation Monte Carlo gases
  - Particle-in-Cell
- Requires irregular mapping of data and computations
  - Computational chemistry, irregular meshes
  - Neighbor-list computations

Example Applications

HPF Meeting (NPAC Technical Report SCCS 692)
guide the HPF-2 process.
The goal of high-level, portable high
features are genuine application requirements.
Underneath the laundry list of desired HPF-2
Significance

HPF Meeting (NPAF Technical Report SCCS 692)
High Performance Fortran Applications

- 2D Potts Model Simulation using Metropolis Hebbath
- CFD Pipe Flow Simulation in 2d
- Spanning Percolation Cluster Generation in 2d
- Monte Carlo Integration for Stock Pricing
- Accept/Reject for Gaussian Random Number Generation
- Convolution in 2d
- NAS CG Benchmark - Conjugate Gradient Solver
- NAS MG Benchmark - Regular Multigrid Solver
- NAS IS Benchmark - Integer Sorting
- NAS EP Benchmark - Tabulation of Random Numbers
- Fast Fourier Transform in 2d
- N-Body Molecular Dynamics
- Elliptic Equation Solution by ADI and Gauss-Seidel

Mini-Applications and Applications Collected
Surfaces

- Monte Carlo Simulation of Dynamically Triangulated Random
- Modified Simplex N-PAC Benchmark
- Simplex N-PAC Benchmark
- N-Body N-PAC Benchmark
- Integration Computation or Pi N-PAC Benchmark
- Laplace Solver N-PAC Benchmark
- Gaussian Elimination N-PAC Benchmark
- FFT N-PAC Benchmark
- Electromagnetic TM Code
- Electromagnetic TE Code
- NAS LU Benchmark – LU Decomposition
- NAS SP Benchmark – Scalar Pentadiagonal
- NAS FT Benchmark – Fourier Transform
- NAS BT Benchmark – Block Triangular
- 2D Binary Phase Quenching of Cahn-Hilliard-Cook Equation
Molecular Dynamics (MolDyn)/Non-bonded Force with Cut-off

ASA – Accessible Surface Area calculation

Barnes-Hut

Van Leer/Prather Advection for Atmospheric Transport

Segmented Bintonic Sort

Wolff Monte Carlo Simulation for Spin Models

Swendsen-Wang Monte Carlo Simulation for Spin Models

Metropolis Monte Carlo Simulation for Spin Models

Block QR

Block Cholesky Decomposition

Block LU using SDOT

Block LU using SAXPY

Block LU using GAXPY

Shallow Water Climate/Weather Model

Monte Carlo Simulation of Fixed Triangulation Random Surfaces
• SPLE - Sparse LU Factorization
• FFT: Fast Fourier Transform (VIEWAS version)
• Out-of-Core Matrix Transposition
• Airshed simulation
• Multibaseline stereo
• Narrowband tracking radar
• FFT: Fast Fourier Transform (TASK version)
• Task parallel (these four codes from CMU/Ex)
• Fock Matrix Construction
• Flame Simulation
• Sparse Cholesky Factorization
• DMC (Direct Simulation Monte Carlo) method
• Biniz - Vortex Dynamics
• Multigrid (MG)

EULER: A Multimaterial, Multidisciplinary, 3-D Hydrodynamics Code
Thanks to

LONG LIST of contributors online... (including much

Syracuse

Maryland

for the HPFF)
Specific enough?

Anecdotes and "war stories" tend not to be

digest by non-domain expert

actually help as they tend to be far too big to

Example codes? (full applications don't

How can this be quantified/qualifyed?

User Experience
Company)

to hack PVM code into the application. Other Aerospace
limited to regular (load balanced) problems and that we will need
compiler on our workstation clusters, but we are concerned it is
...we believe we will want to use HPF when we get an actual
...will it become a real standard? Then we will use it; ‘CFD ISV.

ISV.

pain of going from 66 to 77”, major Oil Reservoir Simulation Code
missings about Fortran 90, let alone HPF – we remember the
Contractor.

“want to use it, but where is the real compiler?”, Defense
Aerospace Company.

“want to use HPF, but only if it does everything F90 does”,
Office)
planning to port to HPF when available” (UK Meteorological

Some (Industrial) Potential-User Comments:

HPF Meeting (NPAR Technical Report SCCS 692)
expressing the same thing
but not the syntax (problem of several ways of
lots of FAQ, suggests that it is easy to learn the ideas

"wish it was more widely available",

Edinburgh Student
"Easier to learn and remember than message passing",

Student
"Quicker to get simulation code written, Syracuse"

Some (academic) user comments
High Performance Fortran Applications

- Talks and lectures on HPF and an On-line HPF Tutorial;
- Parallel computing issues;
- List of papers and books on HPF, Fortran90 and associated
- Issues of relevance to HPF and HPF+
- List of generic example applications codes with discussion of
- Fortran.
- List of industrial and academic application areas with an indication
  of appropriate software including suitability of High Performance
  Fortran.
- Links to HPF material on the Web at other sites — (contributed
  links welcome)
- (Incomplete) List of available Compilers;

Contents of the "HPFA" Web Package
Demand and potential demand for real compilers exist.

- More example codes...
  (any volunteers?)
- Increase the outreach process...
- Requirement?
  Can we identify any obvious priorities from user
deficiencies in HPF being addressed by HPF-2...

Conclusions:
Paul Havlak (havlak@cs.umd.edu)

Maryland "HPF Motivating Applications"

Ken Havlak (havlak@cs.umd.edu)

including Maryland

training material, as well as links to other sites,
HPF Project material at NPAR (codes, documents,
http://www.npac.syr.edu/hpf/index.html

Resources:

More Information & Online Internet