Parallel Library Development at NAG

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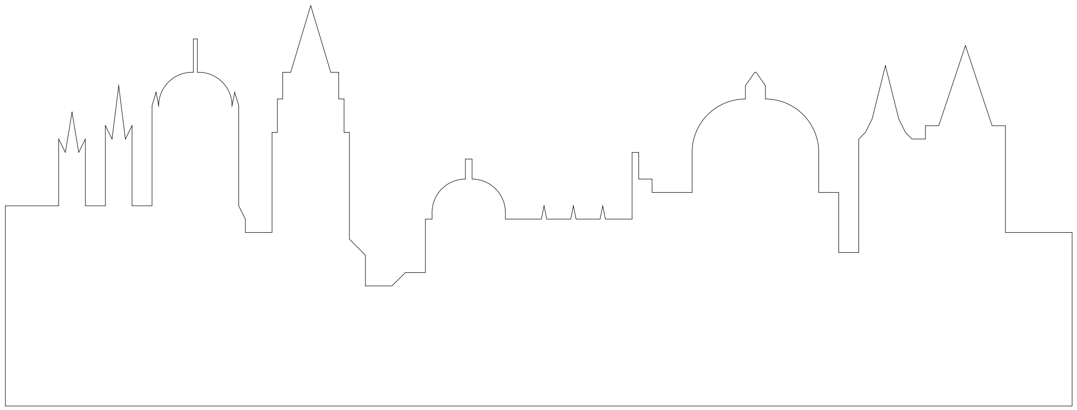

Principal Members of the Development Team:

- Mishi Derakhshan
- Vince Fernando
- Sven Hammarling
- Ken McDonald
- Stef Salvini

Plan of Talk

- Distributed Memory Systems and Portability Base
- A Library for Distributed Memory Systems
- Future Developments

Classes of Systems

- Message passing (Intel Paragon, etc)
- Virtual shared memory (Cray Research T3D, etc)
- Clusters of workstations, (IBM SP-2, etc.)
- Networks of workstations

Basic Assumptions (1)

- Fortran 77 (upgrade path: Fortran 90, HPF)
- SPMD model of parallelism
- Message passing
- Underlying Topology: 2-dimensional logical grid

Basic Assumptions (2)

- Communication Mechanism: BLACS, either native or based on PVM, for **portability** (upgrade path: MPI, HPF)
- Data distribution and Results Collection are the responsibility of the user.
- Minimum dependence on PVM
- Designed with HPF in mind

Library Components

- Numerical software
- Documentation
- Test software to ensure efficient and correct porting
- Example programs

Standards have been defined for all components.

Library Contents (1)

Mark 1 of the Library is virtually completed

- Dense Linear Algebra. Most routines derived from ScaLAPACK
- Iterative Solvers, both for symmetric and unsymmetric systems (CG, SYMMLQ, RGMRES, TFQMR, Bi-CGSTAB).
- 1-, 2- and multi-dimensional quadrature
- Non-linear least squares minimization

Library Contents (2)

- Random numbers generators
- Input/output of matrices and their distribution.
- Distribution of matrices
- Tasks management (task spawning, etc)
- Auxiliary routines (BLAS, PBBLAS, error handling, etc.)

Calling the Parallel Library

```
*   .. call the NAG initialisation routine ..
    CALL nagspawn( ... )
    :
    CALL D01GCFP( ... )
    :
    CALL F07ADFP( ... )
    :
*   .. call the NAG clean-up routine
    CALL nagexit( ... )
```

Future Developments

- Implementation using MPI
- Our Fortran 90 and Parallel Library to merge into an HPF development activity: single source
- Extension of the Library to other algorithms and areas

Parallel Library Strategy – Summary