Preface

In 1984 W. J. Cody, an early member of the IFIP Working Group on Numerical Software (WG 2.5), reviewed progress in numerical software during the previous two decades and then identified future challenges posed by the rapid advances in computing technology[1]:

- decline of the local central computing facility
  - isolated from research
  - libraries neglected
- rise of personal computing
  - isolated from everyone
  - poor software
- rise of remote computing facilities
  - good libraries
  - resident specialists

Cody's foresight was remarkable. The establishment of supercomputer centers coupled with development of distributed computing, including the recent development of grid infrastructure, has resulted in users being increasingly dependent on software resources on remote systems.

Indeed, the use of the Internet to bring together providers and users of resources has become commonplace. One of the earliest such tools was Netlib, which started in the 1980's as an email-based application for distributing numerical software. Other services, such as NetSolve (for linear algebra) and NEOS (for nonlinear and optimization problems) have demonstrated the potential of grid-based problem solving environments (PSEs)[2]. Domain specific PSEs, such as Cactus (developed for numerical relativity) and PYRE (developed for shock physics), have been applied outside their original discipline to generate new PSEs and are being extended to exploit grid technology.

The development and deployment of numerical software for grid-based problem solving environments must ultimately be driven by the needs of scientists and engineers. However, the major changes in the computing environment during the past few years and the advances, both anticipated and unforeseen, during the next few years pose new challenges to the numerical software community as it responds to these needs. There is more to making use of a grid-based service than simply knowing its web address. Does the service work reliably? What are its limitations? Can it be combined with other services? There are also opportunities for improving

[1] W. J. Cody, "Second Thoughts on the Mathematical Software Effort: A Perspective", Proceedings of the Symposium on Computational Mathematics – State of the Art – Held at Argonne National Laboratory September 20-21, 1984 in Honor of James H. Wilkinson, ANL/MCS-TM-42, December, 1984.

[2] In this context, the phrase "Grid-Based Problem Solving Environments" is, in many cases, synonymous with "science gateways" or "science portals", nomenclature introduced recently by the grid community.

the ability of applications to use the best numerical software, for example, by simplifying the acquisition and use of high-quality numerical software. The development of numerical software can benefit from the experience of the scientific and engineering communities using and developing new grid-based PSEs, for example, defining interfaces more appropriate for integrating numerical software into grid-oriented applications and exploiting test sets and tools for comparing different methods.

The IFIP Working Conference on Grid-based Problem Solving Environments: Implications for Development and Deployment of Numerical Software was, therefore, planned to bring together four communities:

- users of both grid-based and traditional problem solving environments;
- developers of both grid-based and traditional problem solving environments;
- developers of grid infrastructure; and
- developers of numerical software

for a week of intensive interaction to address issues including, but not limited to:

- accuracy contracts and software services;
- standards for problem specification;
- service models for the use of numerical software;
- using the grid to link numerical and other services together;
- experiences with web-based numerical services;
- application-oriented numerical interfaces such as web portals;
- software deployment issues including updates and bug fixes;
- large data (including data security) and grid-based numerical software;
- grid-based services as an alternative to deployment; and
- evaluation and comparison of both production and research software.

The conference, WG2.5's ninth working conference since 1978, built upon the experience and insights gained during past working conferences organized by WG2.5, in particular, "WoCo4: Problem Solving Environments for Scientific Computing"[3]; "WoCo6 Programming Environments for High-Level Scientific Problem Solving"[4]; and "WoCo8: Software Architectures for Scientific Computing Applications"[5].

The conference was sponsored by IFIP, organized by the IFIP Working Group on Numerical Software and the Center for Advanced Computing Research at the California Institute of Technology in cooperation with the Society for Industrial and Applied Mathematics. The conference was supported by a major contribution from Hewlett-Packard and additional contributions from Intel, Numerical Algorithms

[3] Editors: B. Ford, F. Chatelin; Problem Solving Environments for Scientific Computing; North Holland, Amsterdam; 1987; ISBN 0-444-70254-7

[4] Editors: P. W. Gaffney, E. N. Houstis; Programming Environments for High-Level Scientific Problem Solving; North-Holland, Amsterdam; 1992; ISBN-0-444-89176-5

[5] Editors: R. F. Boisvert, P. Tang; The Architecture of Scientific Software; Kluwer Academic Publishers, Boston; 2001; ISBN 0-7923-7339-1

Group, and Visual Numerics. Caltech's Center for Advanced Computing Research contributed staff effort necessary for planning and implementing the conference.

Twenty one of the twenty seven presentations at the conference have been expanded into papers included in these Proceedings. The presentations were scheduled in topical groups. A feature distinguishing the conference is the question/answer sessions both after each presentation and after a topical group – the discussions in these sessions are included in these proceedings. Two particular contributions are also included. *Observations on WoCo9*, offers a summary of the meeting, from the perspective of the Program Committee Chair, William D. Gropp. Discussions during the conference stimulated Brian T. Smith to prepare a brief paper, *Future Directions for Numerical Software Research*, emphasizing the need for "software that evaluates the accuracy of the computed results or more importantly the sensitivity of the numerical results to the data and the platforms on which the computation occurs". Abstracts, slides from most presentations, and other information about the conference can be accessed at http://www.nsc.liu.se/wg25/woco9/.

The success of the conference was the result of the Program Committee's guidance and selection of speakers; therefore, we wish to thank: William D. Gropp; Dennis Gannon; Jennifer Schopf; Masaaki Shimasaki; Michael Thuné; and Anne Trefethen. We also wish to thank the members of WG 2.5 who contributed nominations of speakers and participants. We thank the speakers for their efforts to delineate and address the challenges to the numerical software community by the rapidly emerging and changing grid technology and the participants for their insightful questions that stimulated discussions throughout the week. The session chairs and discussants deserve recognition for the difficult task of maintaining the conference schedule while stimulating discussion and recording the questions and answers included in these proceedings. The staff of the Center for Advanced Computing Research at the California Institute of Technology, Sarah Emery Bunn, Santiago Lombeyda, Charles Chapman, and Susan Powell, provided excellent support for the conference planning and implementation.

We thank Ronald F. Boisvert, WG 2.5 Chair, for his support and guidance during the conference planning. We especially thank Brian Ford, Conference Deputy Chair, for his assistance from the earliest planning through the conference implementation to the preparation of these proceedings. Patrick Gaffney, the principal editor of these proceedings, deserves special thanks and acknowledgement for his continuing and persistent efforts to obtain and prepare the papers and discussion dialogues for these proceedings.

Finally, I wish to thank my wife, Doris M. Pool, for her assistance both before and during the conference and for her patience during the months prior to the conference when a multitude of tasks for our new home near Prescott were "temporarily delayed".

James C. T. Pool
Conference Chair