

## GOOSEPACK: A Paradigm for the Parallel Solution of Method of Lines Problems Using Preconditioned Krylov Methods on Distributed Memory Computers

*This paper considers the solution of method of lines problems on distributed memory parallel computers. The approach taken is to base the solution on high quality ordinary differential equation (ode) and spatial differentiation software in conjunction with preconditioned iterative methods for the solution of the associated systems of linear equations. A model based on several well-known mathematical software packages is described. In addition, the manner in which the model has been implemented on a network of serial machines using a well-known message passing protocol is described.*

### 1. Introduction

The numerical method of lines (NUMOL) is a proven and effective way in which to solve systems of partial differential equations [16]. We interpret NUMOL as the use of appropriate spatial differentiation methods in conjunction with high quality adaptive stiff ode solvers. Several such ode solvers have been available for some time now. These solvers include DDRIV3 [8], LSODE [7], LSODES [7], and VODE [1] (and others).

Each of these solvers uses a modified Newton iteration to solve the systems of nonlinear equations which arise in the solution of the corrector equations [3]. Each forms or approximates the Jacobian matrix for the system of odes. The corresponding Newton iteration matrix is then formed and LU factored. The resulting factorization is used subsequently to solve systems of linear equations during the Newton iteration. (Refer to [4] for a discussion of the details of these issues.) Variants of Gaussian elimination are used to accommodate the structure of the Jacobian matrix (*e.g.*, banded, or sparse systems).

Formation of the Jacobian matrix, LU factorization of the iteration matrix, and the subsequent linear equation solutions account for most of the execution solution time and computer storage required by the solvers (see [13] for an illustration). Previous experiments demonstrated that significant speedups are possible by using parallel techniques for the Jacobian formation and Gaussian elimination. The parallel solution of dense systems and sparse systems on shared memory parallel computers was considered in [9,10,13]. The parallel solution of dense systems on distributed memory computers was considered in [11,14]. As in [5], this paper considers parallel Krylov solutions on distributed memory machines.

Due to the growing interest in the solution of huge systems of odes (for example, those resulting from the use of NUMOL for problems requiring a detailed spatial resolution), serial variants of LSODE and VODE were developed. The variants replace the use of Gaussian elimination techniques with the use of iterative linear equation methods, specifically preconditioned Krylov methods [2]. LSODPK [2] and VODPK [2] represent the current state-of-the-art for this approach. Another well-known solver DASPK [12] implements preconditioned Krylov methods for the solution of differential-algebraic equations. A parallel version of DASPK is now available and similar parallel versions of LSODPK and VODPK are anticipated.

### 2. GOOSEPACK

To provide a prototype code based on parallel Krylov methods for distributed memory computers, a solver GOOSEPACK which is based on DDRIV3 was developed. The objective was to develop a parallel Krylov solver which conveniently allows experimentation with different iterative methods and different preconditioners. DDRIV3 was chosen as the ode solver to be used since its "USERS" option allow the user to maintain complete control of the Jacobian and linear algebra related calculations without modifications to the ode solver. However, we emphasize that the methods and software used in GOOSEPACK are applicable to other ode solvers like those cited above.

Modules from the DSS/2 method of lines package [16] are used to perform the necessary spatial discretizations. In order to provide a tool which could be used on networks of serial computers, a widely-used message-passing

Subroutines	Description
FORMJ, FORMP	optional Jacobian and preconditioner setup calculations
PRECONL, PRECONR	left and right preconditioner calculations
MATVEC	matrix free approximations for matrix–vector multiplications
PDNRM2, PDNMAX, PDSUM	parallel norm and inner product calculations

Figure 1: Required Subroutines

MAIN DDRIV3		
DERIVS	USERS PVM3	(STUB)
FORMJ, FORMP	PIM	(STUB)
DERIVS	GMRES	
PRECONL, PRECONR (STUB)	MATVEC DERIVS (STUB)	PDNRM2, PDNMAX, PDSUM

Figure 2: GOOSEPACK Organization

protocol [6] was incorporated. (Future versions of GOOSEPACK will incorporate other well-known message passing protocols.) This approach allows users to perform preliminary studies of the effects of different parallel methods. GOOSEPACK implements parallel iterative methods from the PIM [5] package. Use of [6] facilitates experimentation with different iterative linear methods, preconditioner methods, and parallel message passing protocols and provides a means of conveniently studying the effect of crucial solution parameters (*e.g.*, the maximum allowable Krylov subspace dimension).

In order to minimize changes to DDRIV3 itself, all parallelism is invoked from within the user-supplied USERS subroutine. When an iterative method is used in this context, two crucial sub-steps are matrix–vector multiplications or matrix free finite difference approximations for matrix–vector multiplications, and inner–product computations. Norm calculations are required also.

In addition to providing a DERIVS subroutine to define the system derivatives, the user may supply several subroutines if is not desired to use the default subroutines to perform various calculations. GOOSEPACK contains user replaceable stubs at crucial solution points in order to allow the user to experiment with alternate methods and software. The relevant subroutines are summarized in Figure 1.

The overall organization of GOOSEPACK is depicted in Figure 2.

The approach used in the development of GOOSEPACK allows the user to control and experiment with all phases (particularly the preconditioner phase!) of the parallel solution as well as study the effect of crucial integration parameters. It has been used to solve a number of interesting problems, results for which will be reported elsewhere. It is anticipated that future versions of GOOSEPACK will include the use of sparse ILU preconditioners; preliminary experiments with such preconditioners from [16] are very encouraging.

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