Linear Algebra Templates Usage

Over the last few years there has been a great deal of activity in developing numerical methods for the solution of nonsymmetric systems. This work has gone on primarily in the numerical analysis community and, as a result, we have seen a number of methods presented in the mathematical literature. The presentation of the methods usually requires considerable effort in making them understandable to the general computational scientist in fields such as physics, chemistry or biology. Hence, these approaches are slow in reaching the general computational practitioner. We have developed the concept of *templates* to help with just this problem and facilitate technology transfer between disciples.

Templates are programs which permit the user to inspect, modify or ignore any desired level of implementation detail. Unlike "black-box" libraries, which encapsulate all details and strictly limit allowable algorithmic options and data structures, templates encapsulate those parts of an algorithm the user is unlikely to want to change, expose details important for performance tuning or guaranteeing adequate convergence, and are able to accept a wide variety of user data structures. By writing most of the template in a "data structure neutral" manner, portability is enhanced. Supporting material includes extensive, decision-tree based tutorials to help the user easily choose the right algorithm and its implementation. With Templates, the algorithms are presented using the same notation in a straight forward manner permitting the user to inspect, modify, or ignore any desired level of implementation detail. Hints on parallelization, use and other practical aspects are provided.

Using templates, we have developed a book entitled "Templates for the Solution of Linear Systems: Building Blocks for Iterative Methods" authored by Richard Barrett, Mike Berry, Tony Chan, Jim Demmel, June Donato, Jack Dongarra, Victor Eijkhout, Roldan Pozo, Chuck Romine and Henk van der Vorst, published by SIAM. This book presents the state-of-the-art in methods of solution for large sparse nonsymmetric systems of linear equations using iterative techniques.

In addition to being available commercially through a publisher, this publication is one of the first books available electronically. (SIAM Publishing is trying an experiment with this book and has allowed the postscript and html files containing the book to be distributed freely over the Internet.)

Recently we asked the people who requested the material for their reaction. Below is a summary of the responses.

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From: Adam.Harris@mayahtt.ca (Adam Harris)

Dear Templates Group,

We use your material, and think it is wonderful. Our application is heat
transfer. Typical problem size is 20,000 nodes. I think it would be very
helpful if you had included in the source code some efficient preconditioning
routines such as ILUT.

Thank you,

Adam Harris
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From: pradeau@euler.mcs.utulsa.edu (Francois Pradeau)

Dear Templates Group members,

I really found your work helpfull and easy to read.
The only little comment I would do deals with the theory in it, which could be maybe a little more developed (Krylov spaces, for example).

Anyway, this publication represents a reference in this field for me, and the softwares proposed with are easy to use.

Best regards,

Francois Pradeau

From: Francois Robin <robinf@alofi.etca.fr>

As a computer scientist, I am not supposed to solve mylself linear systems. But since my work is to help other people to use parallel systems, I try to have some knowledge of basic algorithms. So I have read your book to improve my understanding of the work done by people around me in my company. I keep the book as a precious reference.

Very good book, easy to read. I have not the book with me today but I think that I have found the part on domain decomposition a little to short.

From: Paul Van Dooren <vdooren@decision.csl.uiuc.edu>

I have mainly used the text as a useful source for (old and new) references.
I have also recommended the book to my students who followed a course in linear algebra for systems and control. Problem solving in that course was on artificial data and was only to illustrate the methods (hence small scale : 100 at most)

Paul Van Dooren

From: Zbigniew Leyk <zleyk@maths.anu.edu.au>

For me "Templates" is a very good source of information about iterative methods.

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Yours sincerely,
Zbigniew Leyk

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From: Albert Lerusse <lerusse@cupidon.ltas.ulg.ac.be>

  My application corresponds to the computation of the
  dynamic response of structures containing local nonlineatities
  (dry friction, contact, nonlinear spring,..) by the
  multiharmonic balance method.
  This application is very interresting for mechanic application.

  In the state of art, the larger system treated is a 1500 x 1500 system.

  Your work is very very good and the fact that the book
  is documented by the program is really good.
  The matlab version is very interesting because during developments,
  we generaly start by a program in matlab to test the method so
  we can have exactelly the same algorithm from the starting point
  to the end point due to the fact than  in development we use the matlab code
  and in the fortran code we use the fortran code.
  When someone need information about iterative methods, we say that the first
  job corresponds to get the templates book.
  Thanks you very mush and I hope that you continue like this.

Albert Lerusse

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From: scroggs@wave.math.ncsu.edu (Jeff Scroggs)

I used the templates book for a senior-level undergraduate course on linear algebra as a supplement. I thought the concise presentation of the material was just right for the course--there are plenty of books on details, but this is the only one that I could really call a 'reference'. The material I focused on was the Krylov-based iterative methods (GMRES and CG).

Keep up the good work, and if you are going to change it, may I suggest that you not expand the explanations. The students really appreciated being able to get to the method quickly without having to know a massive amount of background material.

Regards,

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From: <JSANYAL@VAXC.STEVENS-TECH.EDU>

Dear Madam/Sir,

I downloaded the TEMPLATE material from ORNL a few months ago. Let me congratulate you on doing a fine job in compiling all the necessary material in such a compact format. I wanted to use the Conjugate Gradient algorithm. It was presented in a very lucid manner. I finally ended up writing my own code because I was dealing with a 3-D finite difference grid discretized on a seven-point stencil and therefore wanted to take advantage of the banded structure of the matrix. The sample codes were provided in dense storage, but I understand they are meant to be quite general and not problem specific. I was dealing with the solution of a 76 X 76 X 82 grid (x-y-z directions respectively). The text material in the book was very helpful in understanding ther nature of the algorithm and the final form of the SSOR matrix was an added boon. Again, hats off on doing an execellent job.

Suggestions: Writing the matrix multiply routines to suit 5-point and seven point stencils.

Thanks

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From: Thomas H Pulliam <pulliam@rft29.nas.nasa.gov>

I have been using the Templates material extensively. I have used it to study and understand the algorithms better. I an weaving some of the material in a course I teach at Stanford next fall (Into. to CFD) and I have been using code from the Templates lib's in my appliacations.

We are developing and employing Krylov subspace methods to solution of the Euler and Navier-Stokes equations. In work on the compressible and incompressible Navier-Stokes equations. We are using the GMRES, BICGSTAB and other codes coupled with ARC2D and INS2D here at NASA Ames. In 1-D studies using the Templates codes and coupling Newton and Tensor based nonlinear techniques we have meet with excellent success. In multidimensional studies the Templates orginated Krylov based codes are giving us a factor of three or more improvement in efficiency.

System sizes on the order of 500,000 to 1,000,000 are typical.

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From: "John R. Gilbert" <gilbert@parc.xerox.com>

Yes, I FTP'd the book and software as soon as it came out, and then bought a bound version of the book from SIAM at my first opportunity.

1. Experimenting with preconditioners for sparse iterative solvers.

2. As a consultant to Xerox scientists with a variety of applications.

I myself am using only the Matlab codes, and am solving systems of dimension up to about 5000 or so.

I have had to modify the Matlab codes slightly to make efficient use of Matlab's sparse matrix stuff; as supplied they occasionally do things like forming full zero matrices, repeatedly dividing by the preconditioner without factoring it first, and so on. I'd be happy to participate in an effort to make the Matlab codes more useful for large problems in the next edition.

It would be useful to the folks I consult for if the Templates codes included some simple preconditioners, both in Matlab and Fortran.

The book itself is a wonderful resource at all levels. Congratulations to the authors, and special thanks to them and SIAM for the bold experiment of making the book available by FTP with no strings attached.

- John R. Gilbert

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From: David Dobson <David.Dobson@math.tamu.edu>

My main application is linear systems arising from finite element approximation of time-harmonic electromagnetics equations. The matrices are complex-valued and generally non-Hermitian, non-positive semidefinite. Sometimes preconditioners are available.

As large as possible. Right now on my workstation, that generally means 50000 x 50000 is about as large as I'm willing to wait for. I'm currently using a (non-Templates) Orthomin code.

Thanks for the fine work with Templates--you have provided an important resource. I particularly like the format of the book. Good luck with the next edition.

David Dobson
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From: pmiller@pmiller.hdos.hac.com (Peter E. Miller)

Non-stationary deconvolution.

8000 x 16000, sparse, underdetermined, and constrained.

The book is excellent for its description and use of the methods, from the overview level down to the computational details. It showed me, for the first time, the relationship among the approaches from which I could directly compare the utility of each for my application.

I would like to see more templates books.

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Peter E. Miller

From: Wolfgang Hartmann <saswmh@unx.sas.com>

Dear friends at SIAM:
I like your book very much! And in future I want to use it for implementing new software for my company (SAS Institute). I'm in the process of writing a set of subroutines for large sparse linear systems. The size of the problems depends on the user specified application. But we need to switch automatically from dense to sparse without telling the user about it. I will certainly buy your new edition (the first one I've got unexpectedly free by email).
Thanks again for you valuable work,
Wolfgang Hartmann

From: mundrane@jove.rutgers.edu (Michael Mundrane)

Sorry about the delay. I found the Templates material extremely useful. My current research involves numerical calculation of convective flows and have run simulations in 2D and 3D (very slow). The 3D simulation consisted of 48\^3 and I was attempting to get 64\^3 simulations and was extremely disappointed with throughput. The "templates" information is just one of several alternatives I am dabbling with in my spare time. A really useful piece of work. The CG section is really complete. If you were considering the addition of material, some of the topics in Ch. 5

could be expanded.

M.

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From: mamh@rhea.cray.com (Michael Heroux)

I am sure that the templates are useful to newcomers in this field. However, for anyone who has worked in this area, even for only a short time, it offers little that is new and the topics addressed in the book can be covered by a careful selection of six to ten papers that exist in the literature. To really improve the value of this project, I would suggest the following ideas:

- Provide sophisticated implementations of the basic iterative schemes. With the exception of perhaps GMRES and QMR with look-ahead, the schemes as described in the Templates are very simple to implement and are not of great value since even a novice can implement them in a short time. However, if the templates provided sophisticated, robust implementations in the spirit of LAPACK, they would be of great value, even to people who are experts in the field. Just a few examples of features that could be added are:
  - Provide the capability to estimate spectral properties.
  - Provide schemes to reorthogonalize if near linear dependence is detected.
  - Provide mechanisms to handle families of matrices and RHS, e.g., use the Krylov vectors from one RHS to "precondition" the initial guess for the next RHS.
  - Provide sophisticated stopping criteria which guarantee that the *true* residual is being reduced.

  I realize that these are difficult tasks, but they would add tremendous value to the Templates in much the same way that careful attention to numerical properties in the EV and SVD routines has made LAPACK so valuable.

- A second general topic would be to include some of the more popular preconditioners using common data structures. For example, incomplete Cholesky with fill-in and diagonal shifting, or Incomplete LU.

- A final item would be a thorough discussion of the use of iterative schemes, especially the potential pitfalls, For example:
  - The loss of orthogonality and the dangers of too many iterations (and therefore the importance of a robust preconditioner).
  - The difference between reducing the pseudoresidual and the true residual, and the relationship to reducing the error in the solution.
  - The importance of preserving the *original* operator, especially for nonsymmetric highly off-diagonal operators.
  - The context in which an iterative solver is used. In particular, the fact that most simulations generate families of problems via some nonlinear or time dependent process.

  In order for iterative schemes to be truly useful in "real world problems", these issues must be understood and addressed by the user.

These general topics are what I can think of at this time. I would be happy to have an ongoing discussion about these items. Please feel free to contact me.

Sincerely,

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From: Stuart Norris <norris@cfd.mech.unsw.OZ.AU>

Yes. I have implimented CG, CGS, BiCG and BiCGSTAB for 2D and 3D Finite Volume meshes. These are working on serial and parallel platforms, with Jacobi, SSOR and MSI preconditioners (The latter two only on the serial machines).

2D and 3D finite volume code to solve fluid flow problems. I use BiCGSTAB to solve the pressure field.

256x256 2D meshes, 64x64x64 3D meshes (65536 and 262144 equations respectively).

I found the book most useful. Could do with some templates for preconditioners. I am corrently using MSI as a preconditioner for BiCGSTAB, which is a method you don't discuss (SIP and MSI are interesting solvers for Finite Difference methods).

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