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TEMPEST USERS' GUIDE

by

Alfred Wong

Memorandum No. UCB/ERL M94/64

14 July 1994

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ELECTRONICS RESEARCH LABORATORY

College of Engineering University of California, Berkeley 94720

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Contributors

This is the third release of TEMPEST. The previous release dates were:

ver1.0 July 23, 1991.

ver2.0 December 31, 1992.

The following people have contributed to TEMPEST:

Original Authors:

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Roberto Guerrieri(ver1.0)

Karim Tadros(ver1.0)

Alfred Wong(ver2.0 and 3.0)

Contributors to earlier releases:

Takeshi Doi(ver1.0)

Eric Hall(Manual Format)

TEMPEST is being developed at the University of California at Berkeley by a student research group on process modeling and technology with Professor Andrew R. Neureuther. The development of TEMPEST has been primarily supported by a SRC/SEMATECH grant, as well as computer time from the Thinking Machines Corporation and the National Center for Supercomputing Applications (NCSA).

An initial *LISP version for the CM-2 architecture was written by John Gamelin and extended and tested by Karim Tadros. Alfred Wong converted the code to C*, added TM polarization, off-axis illumination, and post process image synthesis in version 2.0. In version 3.0, Alfred Wong added three-dimensional analysis capabilities on the CM-5 and linked TEMPEST with SPLAT.

To encourage open exchange of information, TEMPEST and its supporting utilities are available on an as-is basis for a small handling fee. However, there is usually no assistance available for implementing the program or in training users. Although a prompt response cannot be promised, feedback on the program and comments are welcome. Please mail to:

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Conf		

TEMPEST version 3.0

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1.0 Introduction

1.1 Overview

The acronym TEMPEST⁴ stands for "Time-domain Electromagnetic Massively Parallel Evaluation of Scattering from Topography." The computer program solves Maxwell's equations using a time-domain finite-difference algorithm, where the electric and magnetic field nodes are spatially and temporally staggered over a three-dimensional topography of interest. It takes advantage of the inherent parallel nature of electromagnetic wave propagation and is implemented on the computer architecture connection machine 5 (CM-5)⁸. The simulation domain may represent periodic, isolated, or symmetric topography. The algorithm is capable of simulating problems such as scattering from asymmetrical alignment marks, transmission through phase-shifting masks, effects of line-edge profiles in metrology as well as dynamic bleaching of photoresist over arbitrary non-planar, inhomogeneous wafer topographies.

Illumination is assumed to be monochromatic, with the electric field linearly polarized in any user-specified direction. The incident angle can take on discrete values depending on the illumination wavelength and the dimension of the simulation domain. Illumination is assumed to be coherent and can consist of any intensity profile such as that calculated from SPLAT⁹. The steady-state electric fields as well as the magnitudes and phases of diffraction harmonics are found. The photosensitizer concentration is calculated if a layer of photoresist is present. The matrix containing this concentration information can be used in other simulation programs such as SAMPLE⁵ for simulation of resist development. Information on the diffraction harmonics is used to form optical

image profiles in SPLAT⁹. Imaging can be done on the scattered fields (for example, reflected light from alignment marks) or the transmitted fields (for example, light passing through a phase-shift mask).

TEMPEST parses topography information from an input file which can be checked for correctness on a workstation using the pre-processor CHECK. This file can then be transferred using telnet or the unix command ftp to one of the computers facilities offering time on a CM. The input geometry is then loaded onto the processors of the CM and simulated until the electromagnetic field reaches steady-state or, in the case of non-convergence, the simulation domain is excited for a user chosen number of wave cycles. Information on the simulation parameters as well as the diffraction harmonics are written to an output file. Optical image profiles based on the diffraction harmonics can be generated locally on a work station by the program IMAGE2D which calls the simulation program SPLAT⁹. Line plots, contour plots, and/or density plots of the field amplitude, steady-state field, transient field, refractive index and photo active compound (PAC) concentration in any region of the simulation domain can be generated locally using the plotting package PLOTMTV.

The prohibitive expense of high performance computers, such as the CM, causes some concern of availability. However, any user obtaining an account on one of several public access sites around the United States is capable of running simulations from a local work station communicating via the Internet. Appendix B lists several of these sites and the appropriate person to contact for information on how to obtain an account. Note that these sites may have restrictions on the usage of their facilities. Details of the CM can be found in the CM-5 Technical Summary⁸.

1.2 New in Version 3.0

Version 3.0 of the program TEMPEST has several key extensions from the previous version (version 2.0). Three-dimensional problems can be analyzed in addition to two-dimensional problems. Dispersive materials which cause numerical instability in version 2.0 can be modeled in version 3.0. Image synthesis is performed with a link to the simulation program SPLAT. This link enables the study of rigorous electromagnetic simulation with modified illumination, pupil filtering, and arbitrary lens aberrations simultaneously.

In version 2.0, data are available on the magnetic field as well as the electric field, non-steady-state fields and steady-state fields, transient fields, field amplitudes and instantaneous field values, PAC concentration, and the diffraction harmonics. Besides these data, version 3.0 can provide information on the refractive index, the total field, as well as the value of the Poynting vector.

Display of the data has also been changed in version 3.0. The previous version (version 2.0) uses different plotting programs such as DRAWPLOT and MATHEMATICA for different types of plots. In version 3.0, only one plotting routine (PLOTMTV) is used regardless of the data type. This makes the display of data easier for the user.

There is also a slight change in the way one submits a CM-5 job. After telnet or remote login to the partition manager of the CM-5, the user must issue the command **jrun** instead of **cmattach** to access a partition of the CM-5. To run TEMPEST simulations as batch jobs, one uses the command **jsub** instead of the unix command at.

Besides the main electromagnetic fields solver program, TEMPEST version 3.0 includes several auxiliary programs. The program CHECK allows the user to check for possible errors in the input file. The programs AMPHA1D and AMPHA2D allow the user to calculate the amplitude and phase of any electromagnetic field component along any line or plane. IMAGE2D is a routine which calls the simulation program SPLAT for image synthesis. REDUCE2D is used to reduce data volume and to ease output data processing.

1.3 Applications Information

TEMPEST is capable of simulating a number of optical phenomena occurring in photolithography and optical metrology applications. These include bleaching of photoresist over arbitrary topography (e.g., reflective notching), dark-field and bright-field imaging of wafer features (e.g., alignment marks and line structures), generation of image profiles through masks (e.g., reduction phase-shift mask), and calculation of the electric and magnetic fields at all points in the three-dimensional simulation domain at any instant in time. Several studies involving these topics have already been performed, and the user is encouraged to refer to these publications^{2,4,6,7,11,12,13,14}. In general, TEMPEST simulations can be placed into two categories:

- 1. Lithography which involves dynamic changes during exposure, and
- 2. Imaging and scattering analysis.

These categories are distinguished primarily by the desired output. For lithography the desired output is the final PAC concentration. For imaging/scattering purposes the primary output desired are the electromagnetic fields and the diffraction harmonics. These data are used by the program SPLAT to form the bright-field or dark-field images. Details of the image synthesis procedure are described in Section 4.4.1. The other desirable output for an imaging/scattering analysis is the field values in the simulation domain. Line plots, contour plots, surface plots and/or density plots of the transient field, the steady-state field, the total field, the Poynting vector, the PAC concentration and

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the refractive index can be generated. Generation of these plots are described in Section 4.1.5.

1.4 Source Code Information

TEMPEST is written in the C* programming language. The source code is distributed into nine text files. Four header files are also included. The header files are:

definition.h constant definitions
global.h global variable definitions

library.h libraries to include

patchlevel.h version and release date information

The files which contain the source code are:

compute.cscomputes the diffraction harmonicsin.csreads information from the input file

init.cs initialization of variables iterate.cs fields computation by iteration

main.csprogram controlmath.csmathematical functionsmisc.csmiscellaneous functions

out.cs prints simulation results to output files

resist.cs models photoresist bleaching

1.5 About this Manual

Section 1.0	Introduction
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A general overview of TEMPEST is

provided.

Section 2.0 Installation

This section discusses how the simulation program TEMPEST and other auxiliary programs are compiled and installed.

Section 3.0 Tutorial

Two tutorial examples to let the user become

familiar with the commands and procedures

of running TEMPEST are given

Section 4.0 Detail Command Descriptions

Detail descriptions of the commands and input file keywords are presented in this

section.

Introduction

Section 5.0 Useful Hints

Some useful hints for running TEMPEST are

given.

Appendix A Summary of Commands

Important commands are briefly listed.

Appendix B Connection Machine Facilities

Use this section as a reference to connection

machine facilities.

The conventions used throughout this users' guide are as follows:

• Words which are in ALL CAPITAL LETTERS represent programs or shell scripts.

- Words in **bold** letters represent commands to be typed exactly as it appears on the users' guide.
- Words in *italics* represent commands or arguments which can take on different values or character strings.
- Words inside [square brackets] are options to commands which may be omitted.
- Words in the Courier font represent characters in a file or output from programs.
- The string "ws%" represents the unix prompt on a workstation.
- The string "cm%" represents the unix prompt on a partition manager of a CM.

Installation

2.0 Installation

2.1 Resource Requirements

The local computing environment of the user should:

- run unix C-shell
- have a C compiler
- have access to telnet ftp
- have a postscript printer
- have at least 20 mega bytes of disk space available to hold the data files

In addition, it is useful to have X11 windows to display plots of the data by the plotting program PLOTMTV.

2.2 Installation

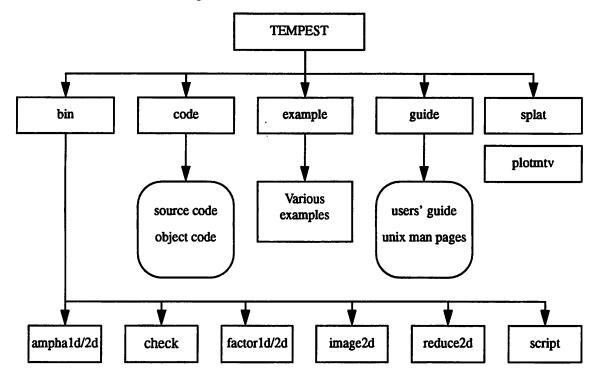
This software package consists of the main program TEMPEST, for use on a CM, as well as other supporting routines to be run on the user's workstation.

- 1. TEMPEST (CM program in C* for electromagnetic simulation.)
- 2. CHECK (Workstation program in C for checking the input file.)
- 3. IMAGE2D (Workstation program in C which calls SPLAT for image synthesis.)
- 4. AMPHA1D and AMPHA2D (Workstation programs in C which calculates the amplitudes and phases of the electromagnetic fields from the instantaneous field values.)
- 5. FACTOR1D and FACTOR2D (Workstation programs in C which scale the axes of plot files.)
- 6. REDUCE2D (Workstation program in C for reducing data file size.)
- 7. PLOTMTV (Workstation program written in C for displaying data files.)
- 8. SPLAT (Workstation program written in C for calculating aerial images.)

To install TEMPEST, please move to a directory (say \$HOME/bin) where TEMPEST should reside. Then insert the tape into the tape drive, and type the following command:

ws% tar xv

After tape reading is completed, which takes about 10 minutes, a TEMPEST directory is created in the \$HOME/bin directory. The programs and shell scripts are organized as follows:



2.3 Compilation

2.3.1 TEMPEST

The electromagnetic simulation program TEMPEST must be installed and run on a partition of the CM. To compile TEMPEST, follow the steps:

- 1. ws% cd \$HOME/bin/TEMPEST/code
- use the unix command ftp or rcp to copy every file in the directory \$HOME/ bin/TEMPEST/code to a directory (e.g., CM_code) on the partition manager of the CM.
- 3. telnet or rlogin to a partition manager of the CM
- 4. cm% cd CM_code
- 5. cm% make

Installation

2.3.2 SPLAT

The program SPLAT can be compiled using make:

- 1. ws% cd \$HOME/bin/splat
- 2. ws% make

2.3.3 PLOTMTV

Compilation of **plotmtv** uses the utility **xmkmf**. Please following the instructions in the file **\$HOME/bin/plotmtv/README.INSTALL**

2.3.4 OTHER ROUTINES

The other routines such as AMPHA1D, AMPHA2D, CHECK, FACTOR1D, FACTOR2D, IMAGE2D, and REDUCE2D can be compiled as follows:

- 1. ws% cd \$HOME/bin/TEMPEST/bin
- 2. ws% makeall

2.4 Testing

When all the programs are compiled, they can be moved to a directory which is contained in the unix variable \$PATH, for example, \$HOME/bin.

To test if the programs are installed properly and the computing environment is proper, please do the following:

- 1. ws% cd \$HOME/bin/tempest/example
- 2. ws% test

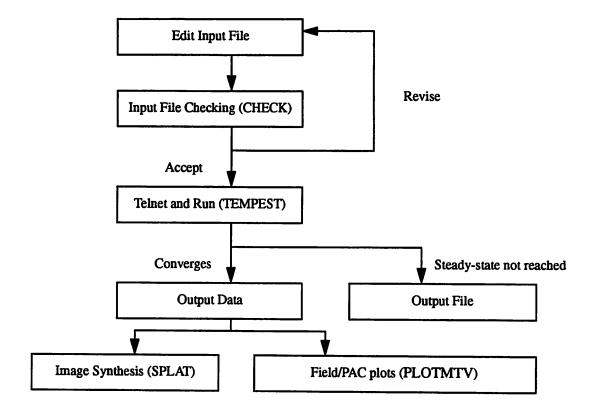
The pictures shown in Figure 1 to Figure 4 of this manual should be displayed on the screen within a few seconds. If a plot is not displayed, check that the \$DISPLAY variable is set properly (ws% setenv DISPLAY host:display) and the machine you are working on is added as an xhost to the work station machine (ws% xhost machine).

3. Follow the examples in Section 3.0 to make sure that all the routines are functioning properly.

3.0 Tutorial

3.1 Overview

The basic steps in running TEMPEST simulation are shown as follows:



A typical simulation takes about 10 minutes to run on the CM-5. However, if a large amount of data (such as a contour plot of a large area) is requested, the simulation time can be as much as one hour.

3.2 Input File to TEMPEST

The input file to TEMPEST contains five types of specifications:

- 1. simulation domain
- 2. illumination
- 3. topography
- 4. analysis (numerical parameters)
- 5. data (output specifications)

The input file to TEMPEST can be given any name and the entries in the input file can occur in random order. (The only exception is that the definition of wavelength must precede the definition of any block property.) The input file to TEMPEST consists of a list of keywords; each keyword may be followed by numbers, words, or other keywords. A detail description of the keywords is found in Section 4.1. Comments can be included in the input file by including the string "/*" before the comment and the string "*/" after the comment.

As a first example, transmission through a convention chrome mask is studied. The input file is located in the directory \$HOME/bin/TEMPEST/example/example1 and is named example1.in. The dimension of the simulation domain is 4.0 μ m by 4.0 μ m by 1.0 μ m. The chrome mask has a glass substrate with a layer of 80 nm thick chrome. The square opening on the chrome has a width of 1.0 μ m on each side. Illumination is assumed to be normally incident at 248 nm, with the electric field linearly polarized in the x-direction. In this study, the transmitted diffraction harmonics are requested to study the transmission characteristics of the mask. In addition to the diffraction harmonics, the transmitted electric field in the x-direction is also requested.

The input file example 1. in is shown as follows:

```
/*
input file name: example1.in
*/
simulation window is 4 by 4 by 1 microns with 256 simulation nodes in the x-
and y-directions and 64 nodes in the z-direction.
*/
x_node 256
y_node 256
z_node 64
x_dim 4.0
y_dim 4.0
z_dim 1.0
periodic
wavelength of 248 nm with 1000 mW/cm^2 of incident flux density normally
incident with the electric field linearly polarized in the x-direction.
*/
wavelength 0.248
intensity 1.0
inc_the 0.0
inc_phi 0.0
rel_ex0 1.0
/*
transmitted harmonics are requested. An inconsistency of 1% in the fields can
```

```
be tolerated, and the maximum number of wave cycles simulated is 300.
*/
transmitted
max_cycle 300
err_tol 0.01
/*
First block is air - index 1.0
*/
block 1
figure rectangle
0.0 4.0 0.0 4.0 0.0 1.0
index 1.0 0.0
end_block
/*
Second block is glass - index 1.5
*/
block 2
figure rectangle
0.0 4.0 0.0 4.0 0.6 1.0
index 1.5 0.0
end_block
/*
Third block is chromium.
*/
block 3
figure rectangle
0.0 4.0 0.0 4.0 0.52 0.6
index 2.5 2.0
end_block
/*
Fourth block is air again.
*/
block 4
figure rectangle
1.50 2.50 1.50 2.50 0.52 0.6
index 1.0 0.0
end_block
Steady-state electric field plots.
*/
plot steady xyplane
                        0.00 e x
                                      position 0.0
                                                      4.0
                                                            0.0
                                                                 4.0
                                                                       0.5
example1.ex.xypln.000
plot
      steady
                        0.25 e x
                                                0.0
                                                            0.0
              xyplane
                                      position
                                                      4.0
example1.ex.xypln.250
```

```
steady yzplane
                      0.00
                                                               2.0
plot
                              x position
                                           0.0
                                                     0.0
                                                          1.0
example1.ex.yzpln.000
     steady yzplane
                      0.25
                                                     0.0
plot
                                  position
                                           0.0
                                                4.0
                                                          1.0
                                                               2.0
example1.ex.yzpln.250
```

3.3 Checking the Input File

Since computation time on the CM is expensive, it is desirable to ensure that the format of the input file is correct before submitting it to be simulated. The routine CHECK checks an input file for possible errors. If the input file contains errors such as incorrect keywords, the program notifies the user of the mistake.

To check the input file example 1. in, type the command:

ws% check example1.in

With this command, the following is displayed, indicating that there is no error in the input file *example1.in*:

```
C H E C K
ver3.0
94/07/14
```

```
Reading input file [example1.in]...

Done reading input file [example1.in].
```

No error detected. CHECK executed successfully.

3.4 Running Simulations

With no error messages from the checking routine CHECK, the input file is in the correct format and TEMPEST can be run. To execute the program TEMPEST, the user must be attached to a partition of the CM. A partition controls a certain number of nodes. The actual number of nodes each partition can control depends on the size of the CM. For instance, the CM-5 of the National Center for Supercomputing Applications (NCSA) at Urbana-Champaign, Illinois has 512 nodes (a 512-node machine) divided into units with 256, 128, 64, and 32 nodes. When one attaches to the CM through a partition manager, one tells the partition manager the number of nodes needed. The number of nodes requested is related to the problem size. In TEMPEST, the minimum number of nodes required is given by the product of the simulation nodes in the x-, y- and z-directions divided by the number 65536.

The first step to attach to a CM is to telnet or remote login to a partition manager of the CM. For example, to login to user "tempest" on the NCSA machine, type the following command:

ws% rlogin cm5.ncsa.uiuc.edu -l tempest

After logging into the partition manager, the user can request to attach to a partition by:

cm% jrun

The machine then asks several questions as follows:

```
Number of processors (32)? 64
Estimated cpu time (5min)? 15
Estimated memory (32M)? 1.5G
Job id is 94080.
[Type ~^B to disconnect, ~^C to kill. Waiting for resources.]
```

In this example, 64 nodes and 1.5 GBytes of memory are requested. The partition manager indicates that there is no free space on the CM-5 at the moment and the process has to wait. To check for the availability of the different partitions, use the command

cm% jstat

This command displays all the users who are currently using the CM-5:

```
USER JID MACH SERV PROCS TIME MEM STATUS COMMAND
tempest 94080 cm5 64 15:00 512M Que dwn /bin/csh
jbokor 94079 cm5 32 5:00i 32M Que dwn /bin/csh
blee 94071 cm5 cm5b 32 11:46? 53.4M Running trial4/gup4
afreeman 94066 cm5 cm5a 32 0:00? 0 Exiting /bin/csh
joannop 94046 cm5 cm5c 64 19:18? 590M Running si111-7/si111-dyn1
bernardo 94011 cm5 cm5d 128 98:55? 731M Running ammonia/lj/elmo_lj
fchen 93950 cm5 cm5a 32 59:44? 476M Running yeeinv2d/sfinv2d
sadayap 93117 cm5 cm5e 256 68:50? 550M Running kaushik/perms/datascript.256
```

The line which starts with "tempest 94080" (the first line) indicates that the process is sitting in the queue. When the queue finally becomes free, we can gain access to the connection machine.

```
[Connected to cm5e.ncsa.uiuc.edu /dev/ttyp2.]

*** Job csh (94080) procs 256, mem 1.5G, cpu 1hr, server cm5e:0

*** tempest /bin/csh started on Sun Jul 3 16:59:30 1994
```

We are now ready to run TEMPEST. There are two arguments for the program TEMPEST. The first argument is the input file name and is *example1.in* in this case, and *example1.out* is the name of the output file. The output file is the file to which information on the diffraction harmonics and simulation parameters is written.

```
[Connected to cm5e.ncsa.uiuc.edu /dev/ttyp2.]
*** Job csh (94080) procs 256, mem 1.5G, cpu 1hr, server cm5e:0
```

```
*** tempest /bin/csh started on Sun Jul 3 16:59:30 1994
cm5e:/nfs/cm5/scratch3/tempest [51]% tempest example1.in example1.out
TEMPEST
ver3.0
94/07/14
Start simulation...
Reading input file [example1.in]...
Done reading input file [example1.in].
Initializing parameters and variables...
Warning:
Minimum number of simulation nodes per wavelength for the topography is 6.35,
fewer than 15. Simulation result may be inaccurate.
Done initializing parameters and variables.
Start iteration...
Period #11:
1st try: 91.59% converged.
Period #12:
1st try: 93.15% converged.
Period #13:
1st try: 91.98% converged.
Period #14:
1st try: 95.50% converged.
Period #15:
1st try: 97.46% converged.
Period #16:
1st try: 99.22% converged.
Period #17:
1st try: 99.02% converged.
Period #18:
1st try: 98.63% converged.
Period #19:
1st try: 100.00% converged.
Period #20:
1st try: 100.00% converged.
2nd try: 98.83% converged.
Period #21:
1st try: 100.00% converged.
2nd try: 100.00% converged.
Period #22:
1st try: 100.00% converged.
2nd try: 100.00% converged.
3rd try: 100.00% converged.
Converges after 22 periods.
```

```
Done iteration.

Writing plot file [example1.ex.xypln.000]...
Done writing.

Writing plot file [example1.ex.xypln.250]...
Done writing.

Writing plot file [example1.ex.yzpln.000]...
Done writing.

Writing plot file [example1.ex.yzpln.250]...
Done writing.

Calculating diffraction efficiencies...
Done calculating diffraction efficiencies.

Writing to output file [example1.out]...
Done writing.

Simulation successful. Thank you.
```

When the program finishes execution, we need to detach from the CM. To do so, do the following:

```
cm5e:/nfs/cm5/scratch3/tempest [52]% exit
cm5e:/nfs/cm5/scratch3/tempest [53]% *** Job terminated at Sun Jul 3
17:16:41 1994
*** exitcode = 0000
*** procs 256, mem 1.56G, cpu 7.77min
***
```

Five data files are generated for this simulation:

- 1. example 1. out (output file which contains information on the diffraction efficiencies)
- 2. example 1.ex.xypln.000 and example 1.ex.xypln.250 (electric field plots across an xy-plane in PLOTMTV format)
- 3. example 1.ex.yzpln.000 and example 1.ex.yzpln.250 (electric field plots across an yz-plane in PLOTMTV format)

These files can be transferred to be processed on a workstation by the file transfer program ftp or the remote copying command rcp.

3.5 Output Data

3.5.1 Output File

The output file of TEMPEST contains information on the simulation parameters, such as the spatial and temporal discretization values, and recapitulates some of the input parameters. If steady-state is reached and the user requested so, information on the diffraction harmonics is written to the output file as well. This information can be used to synthesize the optical image profile of the structure using the image synthesis program IMAGE2D which calls the simulation program SPLAT.

The output file generated, *example1.out*, is shown below. It summarizes the topography information and numerical parameters and contains information on the diffraction harmonics.

TEMPEST

ver3.0 94/07/14

University of California, Berkeley

Miscellaneous Information:

Input file name: example1.in
Output file name: example1.out

There are 4 plot files:

- 1. Steady-state field example1.ex.xypln.000
- 2. Steady-state field example1.ex.xypln.250
- 3. Steady-state field example1.ex.yzpln.000
- 4. Steady-state field example1.ex.yzpln.250

Total time elapsed: 4.7165e+02 second

CM busy time: 60.59% CM idle time: 39.41%

Process Parameters:

Freespace wavelength: +2.4800e-01 um

Incident theta: +0.0000e+00
Incident phi: +0.0000e+00
Refl abs theta 1: +0.0000e+00
Refl abs theta 2: +4.1345e-02
Tran abs theta 1: +0.0000e+00
Tran abs theta 2: +6.2040e-02

```
Incident relative Ex: +1.0000e+00
 Ey: +0.0000e+00
Incident cosine Ex: +1.0000e+00
 Ey: +0.0000e+00
 Ez: +0.0000e+00
 Hx: +0.0000e+00
 Hy: -1.0000e+00
 Hz: -0.0000e+00
 Kx: +0.0000e+00
 Ky: +0.0000e+00
 Kz: -1.0000e+00
Illumination intensity: +1.0000e+00 mW/cm2
Mask file name: None
Topography:
The structure is assumed to be periodic.
x dimension: 4.0000e+00 um
y dimension: 4.0000e+00 um
z dimension: 1.0000e+00 um
Index at north boundary: 1.5000e+00 0.0000e+00
Index at south boundary: 1.0000e+00 0.0000e+00
Number of building blocks: 4
Block 1:
 index (+1.0000e+00 +0.0000e+00)
 eps (+1.0000e+00 +0.0000e+00)
 eta (+3.7673e+02 +0.0000e+00)
 cond (+0.0000e+00)
 fig rectangle
 xl xh 0.0000e+00 4.0000e+00
 yl yh 0.0000e+00 4.0000e+00
 zl zh 0.0000e+00 1.0000e+00
Block 2:
 index (+1.5000e+00 +0.0000e+00)
 eps (+2.2500e+00 +0.0000e+00)
 eta (+2.5115e+02 +0.0000e+00)
 cond (+0.0000e+00)
 fig rectangle
 xl xh 0.0000e+00 4.0000e+00
 yl yh 0.0000e+00 4.0000e+00
 zl zh 6.0000e-01 1.0000e+00
Block 3:
 index (+2.5000e+00 +2.0000e+00)
 eps (+2.2500e+00 +1.0000e+01)
 eta (+9.1885e+01 +7.3508e+01)
```

```
cond (+6.7251e+05)
 fig rectangle
xl xh 0.0000e+00 4.0000e+00
yl yh 0.0000e+00 4.0000e+00
 zl zh 5.2000e-01 6.0000e-01
Block 4:
 index (+1.0000e+00 +0.0000e+00)
 eps (+1.0000e+00 +0.0000e+00)
 eta (+3.7673e+02 +0.0000e+00)
 cond (+0.0000e+00)
 fig rectangle
xl xh 1.5000e+00 2.5000e+00
vl vh 1.5000e+00 2.5000e+00
 zl zh 5.2000e-01 6.0000e-01
Computational parameters:
Distance between nodes (dx): 1.5625e-02 um
Simulation grid: 256 x 256 x 64
Minimum nodes per wavelength: 6.35
Time increment (dt): 2.9544e-17 second
Iterations per period (wave cycle): 28
Convergence information:
Wave cycles before convergence check: 10
Maximum iteration wave cycles: 300
Error tolerance: 1.00%
Number of periods for convergence: 22
Transmitted diffraction efficiencies:
Number of diffracted orders: 16 16
 Real Imag
order[ +0 ][ -3 ]: +5.037091e-05 -1.923219e-02
 -2.716657e-05 -1.102946e-05
 -2.739282e-05 -1.126659e-05
 -8.187038e-06 +1.875915e-02
order[ +0 ][ -2 ]: +1.830793e-03 +3.778544e-02
 +4.256049e-05 +2.094013e-05
 +4.297282e-05 +2.133218e-05
 -1.989200e-03 -3.747990e-02
order[ +0 ][ -1 ]: -5.006125e-03 -5.188354e-02
 -3.576368e-05 -1.723806e-05
```

```
-3.631501e-05 -1.741823e-05
 +5.449582e-03 +5.185812e-02
order[ +0 ][ +0 ]: +7.808192e-03 +5.096931e-02
 +9.865538e-06 +5.952744e-06
 +1.003706e-05 +6.072602e-06
 -7.720337e-03 -5.192857e-02
order[ +0 ][ +1 ]: -4.367713e-03 -5.192599e-02
 +2.185255e-05 +8.608084e-06
 +2.218210e-05 +8.654256e-06
 +4.810850e-03 +5.190511e-02
order[ +0 ][ +2 ]: +9.023458e-04 +3.779706e-02
 -4.188506e-05 -2.162569e-05
 -4.227937e-05 -2.203745e-05
 -1.067477e-03 -3.749463e-02
order[ +0 ][ +3 ]: +7.577330e-04 -1.920048e-02
 +3.816728e-05 +2.329560e-05
 +3.857693e-05 +2.368192e-05
 -6.985012e-04 +1.872935e-02
Transmitted energy: 5.21%
Total refl and tran energy: 30.58%
```

3.5.2 Image Synthesis

Based on the information of the diffraction harmonics contained in the output file, the optical image profile of the simulated structure can be synthesized given the characteristics of the optical system, including the numerical aperture (NA), partial coherence factor, and the magnification factor. Since TEMPEST assumes coherent illumination, partial coherence is modeled by Hopkins' approach¹. Two assumptions are made:

- 1. The magnitudes of the diffraction efficiencies are independent of the angle of illumination.
- 2. The illumination energy is distributed evenly over the illumination cone.

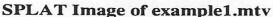
With these assumptions, the intensity at every point in space can be calculated by evaluating the transmission cross coefficients¹. This approach can be used to model bright-field or dark-field optical systems, arbitrary lens aberrations as well as defocus effects.

For the example structure, assume that the optical system is 1X and has an NA of 0.5 and a partial coherence factor of 0.5. The optical signal produced by the chrome mask can be synthesize by the command

ws% image2d example1.out -na 0.5 -sg 0.5 -m 1 -p

where *example1.out* is the output file of TEMPEST. The command **image2d** is described in detail in Section 4.4.1.

With the above command, the image in Figure 1 is displayed on the screen. The data points of the image is written to the file *example1.mtv*.



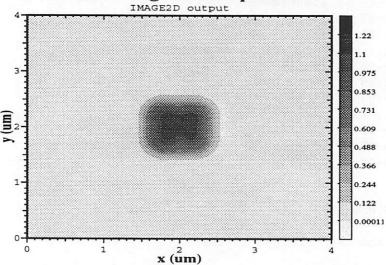


Figure 1 The optical signal created by a 1 μm by 1 μm square opening on a 1X chromium mask. The optical system has an NA of 0.5 and a partial coherence factor of 0.5.

3.5.3 Field and PAC plots

The data files generated by TEMPEST are all in the PLOTMTV format. To plot the data files, simply issue the command

ws% plotmtv file name

For example, to display the data file example1.ex.yzpln.000, type

ws% plotmtv example1.ex.yzpln.000

and the picture in Figure 2 is displayed on the screen.

From the instantaneous values of the fields, it is possible to calculate the amplitude and phase using the routines AMPHA1D and AMPHA2D. For example, from the electric field data <code>example1.ex.yzpln.000</code> and <code>example1.ex.yzpln.250</code>, AMPHA2D can be used to find the transmitted electric field amplitude:

Steady-state E-field in X of yzplane at x=2.000

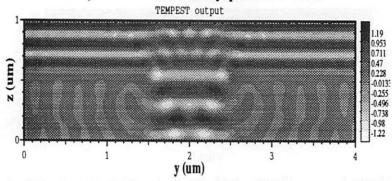


Figure 2 The instantaneous electric field in the x-direction across an yz-plane of the simulation domain. The fields show that the electric field is diffracted as it exits the chromium opening.

ws% ampha2d example1.ex.yzpln.000 example1.ex.yzpln.250 example1.ex.yzpln.amp example1.ex.yzpln.pha

Sometimes raw data files such as *example1.ex.yzpln.amp* are too large. The routine **reduce2d** reduces the size of the data file by taking one out of a few data points from the raw data file. For example, the data file *example1.ex.yzpln.amp* can be processed as follows:

ws% reduce2d example1.ex.yzpln.amp example1.ex.yzpln.amp.red 2 2

The file example 1.ex.yzpln.amp.red contains one datum out of two data points in example 1.ex.yzpln.amp in both the x- and y-directions.

A plot of the file *example1.ex.yzpln.amp.red* using PLOTMTV is shown in Figure 3.

3.6 Example 2: Photoresist Exposure

In the second example, the image synthesized from the first example is used to expose a layer of photoresist deposited over a stepped substrate. The volume of the simulation domain is 4 μ m by 4 μ m by 1 μ m. The ABC parameters of the photoresist is (0.51, 0.031, 0.013). 100 mJ/cm² is deposited onto the photoresist. Bleaching of the photoresist is considered by breaking up the total exposure dose into five steps.

Amplitude Plot REDUCE2D output 1 1.39 1.25 1.11 0.974 0.835 0.696 0.557 0.418 0.07702

Figure 3 Electric field amplitude transmitted through a chromium mask. The data file is generated by the routine AMPHA2D.

y (um)

3

3.6.1 Input File

The input file named example2.in is shown below.

```
input file name: example2.in
volume of simulation is 4 by 4 by 1 microns with 256 nodes in the x- and the
y-directions, and 64 nodes in the z-direction.
*/
x_node 256
y_node 256
z_node 64
x_dim 4.0
y_dim 4.0
z_dim 1.0
periodic
the incident radiation is monochromatic at 248 nm. The incident field
amplitude profile is taken from the file named "example1.mtv"
wavelength 0.248
intensity 1.0
mask example1.mtv
no diffracted efficiencies are requested.
*/
no_de
```

```
max_cycle 300
err_tol 0.01
/*
first block is air
*/
block 1
figure rectangle
0.0 4.0 0.0 4.0 0.0 1.0
index 1.0 0.0
end_block
/*
second block is photoresist
*/
block 2
figure rectangle
0.0 4.0 0.0 4.0 0.15 0.75
index 1.68 0.02
resist 1.0 0.51 0.031 0.013 100.0 5
end_block
/*
third block is silicon
*/
block 3
figure rectangle
0.0 4.0 0.0 4.0 0.00 0.3
index 4.0 2.0
end_block
fourth block is resist
*/
block 4
figure rectangle
1.25 2.75 1.25 2.75 0.15 0.3
index 1.68 0.02
resist 1.0 0.51 0.031 0.013 100.0 5
end_block
/*
PAC plots are requested
*/
plot pac xyplane position 0.0 2.0 0.0 2.0 0.4 example2.pac.xypln
plot pac yzplane position 0.0 2.0 0.15 0.75 2.0 example2.pac.yzpln
```

3.6.2 Running Simulation

Assuming that the routine CHECK has been applied to the input file and the input file is in the correct format, TEMPEST simulation can be run on the input file *example2.in*.

ws% rlogin cm5.ncsa.uiuc.edu -l tempest cm% jrun

```
cm5:~ [34]% jrun
Number of processors (32)? 64
Estimated cpu time (5min)? 15
Estimated memory (64M)? 1.5G
Job id is 94252.
[Type ~^B to disconnect, ~^C to kill.]
[Connected to cm5e.ncsa.uiuc.edu /dev/ttyp1.]
*** Job csh_94252 (94252) procs 256, mem 1.5G, cpu 15min, server cm5e:0
*** tempest /bin/csh started on Wed Jul 6 19:03:51 1994
cm5e:/nfs/cm5/scratch3/tempest [51]% tempest example2.in example2.out
TEMPEST
ver3.0
94/07/14
Start simulation...
Reading input file [example2.in]...
Done reading input file [example2.in].
Initializing parameters and variables...
Warning:
Minimum number of simulation nodes per wavelength for the topography is 3.97,
fewer than 15. Simulation result may be inaccurate.
Reading image information from [example1.mtv]...
Done reading image information.
Done initializing parameters and variables.
Iterating for energy step 1...
Start iteration...
Period #17:
1st try: 100.00% converged.
Period #18:
1st try: 100.00% converged.
2nd try: 100.00% converged.
Period #19:
1st try: 100.00% converged.
2nd try: 100.00% converged.
```

```
3rd try: 100.00% converged.
Converges after 19 periods.
Done iteration.
Updating parameters in the resist layer...
Done updating parameters.
Total exposure time: 1.209e+01 seconds.
Total dose: 1.209e+01 mW/cm2.
Iterating for energy step 2...
Start iteration...
Period #1:
1st try: 100.00% converged.
Period #2:
1st try: 100.00% converged.
2nd try: 100.00% converged.
Period #3:
1st try: 100.00% converged.
2nd try: 100.00% converged.
3rd try: 100.00% converged.
Converges after 3 periods.
Done iteration.
Updating parameters in the resist layer...
Done updating parameters.
Total exposure time: 2.645e+01 seconds.
Total dose: 2.645e+01 mW/cm2.
Iterating for energy step 3...
Start iteration...
Period #1:
1st try: 100.00% converged.
Period #2:
1st try: 100.00% converged.
2nd try: 100.00% converged.
Period #3:
1st try: 100.00% converged.
2nd try: 100.00% converged.
3rd try: 100.00% converged.
Converges after 3 periods.
Done iteration.
Updating parameters in the resist layer...
Done updating parameters.
Total exposure time: 4.412e+01 seconds.
Total dose: 4.412e+01 mW/cm2.
```

```
Iterating for energy step 4...
Start iteration...
Period #1:
1st try: 100.00% converged.
Period #2:
1st try: 100.00% converged.
2nd try: 100.00% converged.
Period #3:
1st try: 100.00% converged.
2nd try: 100.00% converged.
3rd try: 100.00% converged.
Converges after 3 periods.
Done iteration.
Updating parameters in the resist layer...
Done updating parameters.
Total exposure time: 6.709e+01 seconds.
Total dose: 6.709e+01 mW/cm2.
Iterating for energy step 5...
Start iteration...
Period #1:
1st try: 100.00% converged.
Period #2:
1st try: 100.00% converged.
2nd try: 100.00% converged.
Period #3:
1st try: 100.00% converged.
2nd try: 100.00% converged.
3rd try: 100.00% converged.
Converges after 3 periods.
Done iteration.
Updating parameters in the resist layer...
Done updating parameters.
Total exposure time: 1.000e+02 seconds.
Total dose: 1.000e+02 mW/cm2.
Writing plot file [example2.pac.xypln]...
Done writing.
Writing plot file [example2.pac.yzpln]...
Done writing.
Writing to output file [example2.out]...
Done writing.
Simulation successful. Thank you.
```

```
cm5e:/nfs/cm5/scratch3/tempest [52]% exit
cm5e:/nfs/cm5/scratch3/tempest [53]% *** Job terminated at Sun Jul 3
17:16:41 1994
*** exitcode = 0000
*** procs 256, mem 1.56G, cpu 7.77min
***
```

Three output files are produced in this simulation:

- 1. example2.out (output file which contains information on the simulation run)
- 2. example2.pac.xypln (contours of the PAC across an xy-plane)
- 3. example2.pac.yzpln (contours of the PAC across an yz-plane)

The output file *example2.out* is in a form similar to that of the first example shown in Section 3.5.1, and hence it will not be shown here.

3.6.3 Output Data

To display the PAC contours, again using the plotting package PLOTMTV. For instance, to display Figure 4 on the screen, type

ws% plotmtv example2.pac.yzpln

PAC of yzplane at x=2.000

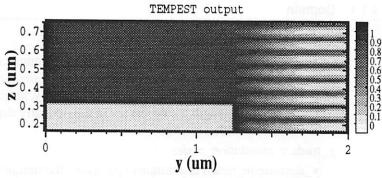


Figure 4 PAC contours calculated by TEMPEST. The photoresist is exposed by the image synthesized in the first example.

4.0 Detail Command Descriptions

4.1 Input File Keywords

The input file to TEMPEST contains five types of specifications:

- 1. simulation domain
- 2. illumination
- 3. topography
- 4. analysis (numerical parameters)
- 5. data (output specifications)

The input file to TEMPEST can be given any name and the entries in the input file can occur in random order. (The only exception is the definition of wavelength must precede the definition of any block property.) Comments can be included in the input file by including the string "/*" before the comment and the string "*/" after the comment. Further, this version (as does the previous version) of TEMPEST performs error checking of the input file and will be able to detect most input errors. The input file to TEMPEST consists of a list of keywords. Each keyword may be followed by numbers, words, or other keywords. The following is a description of the keywords:

4.1.1 Domain

x_node *x_simulation_nodes*

x_simulation_nodes is a number specifying the number of simulation nodes in the x-dimension of the simulation domain. x_simulation_nodes must be a positive number which is a power of 2. Typically, at least 15 simulation nodes per wavelength are necessary in the optically densest material to give accurate simulation results.

y_node y_simulation_nodes

y_simulation_nodes is a number specifying the number of simulation nodes in the y-direction of the simulation domain. y_simulation_nodes must be a positive number which is a power of 2.

The ratio of $y_simulation_nodes$ to $x_simulation_nodes$ must be the same as the ratio between the physical dimensions in y and x.

z_node z_simulation_nodes

z_simulation_nodes is a number specifying the number of simulation nodes in the z-direction of the simulation domain. z_simulation_nodes must be a positive number which is a power of 2. The product of x_simulation_nodes, y_simulation_nodes, and z_simulation_nodes cannot exceed the product of the number of CM-5 nodes and 65536. For example, if one is attached to 256

nodes, then the product (x_simulation_nodes times y_simulation_nodes times z_simulation_nodes) must be fewer than or equal to (256 times 65536).

periodic

keyword **periodic** specifies that the structure under study is a periodic structure. This is the default.

x_dim *x_length*

 x_{length} is the x-dimension of the simulation domain in micro-meter.

y_dim y_length

y_length is the y-dimension of the simulation domain in micro-meter.

z_dim *z_length*

 z_length is the z-dimension of the simulation domain in micro-meter. A constraint is placed on the maximum values of x_length , y_length , and z_length in order to maintain a sufficiently high grid density for simulation accuracy and algorithm stability. Typically, at least 15 simulation nodes per wavelength are necessary in the optically densest material to give accurate simulation results. Therefore, the maximum values of x_length , y_length , and z_length are limited by the number of nodes which is in turn limited by the physical resources of the CM to which the user has access.

isolated

keyword **isolated** specifies that the structure under study is an isolated structure. The default structure type is **periodic**.

1symmetry

if the structure possesses symmetry in one of the dimensions, specify **1symmetry**. The structure is then assumed to be symmetric in the x-direction (with respect to the y-axis). When **1symmetry** is specified, the argument of **rel_ex0** must be 1.0 (the default), and **no_de** should also be specified.

2symmetry

For a structure which is symmetric with respect to both the x- and y-axes, specify 2symmetry. Similar to the case in 1symmetry, the argument of rel_ex0 must be 1.0 (the default), and no_de should be specified.

4.1.2 illumination

wavelength lambda

lambda is the free space wavelength of the incident illumination in micrometer. TEMPEST assumes monochromatic illumination. wavelength must be defined before definition of any block property.

intensity value

value is the intensity of the incident illumination in milli-Watt per centimeter squared. The incident field amplitude is determined from value, which is given by the expression $E = \sqrt{2 \times \text{value} \times 10 \times \text{s}}$ (x) $\times \eta$ where s(x) represents intensity modulation specified by the keyword mask. If there is no intensity modulation, s(x) = 1. The factor 10 is a unit-conversion factor.

inc_the theta_inc

inc_phi phi_inc

The illumination direction is specified by the angles *theta_inc* and *phi_inc*. The direction of propagation of the incident radiation makes an angle of *theta_inc* (in degrees) with the z-axis and an angle of *phi_inc* (in degrees) with the x-axis. The default value for *theta_inc* and *phi_inc* is zero. In the current version, oblique incidence works only for periodic structures. Further, only discrete values of *theta_inc* and *phi_inc* are allowed, corresponding to integral multiples of 360° phase difference between the east-west and north-south boundaries.

rel ex0 ex0

The relative amount of x-polarized electric field is ex0, which is a value between 0 and 1. From ex0, the relative amount of y-polarized electric field is calculated by $ey0 = \sqrt{1 - ex0^2}$. Together with $theta_inc$ (θ) and phi_inc (φ), the directional cosines of \dot{E} , \dot{H} , and $\dot{\kappa}$ are calculated to be

 $(ex0\cos\phi + ey0\sin\phi, -ex0\sin\phi + ey0\cos\phi, ey0\sin\theta)$,

 $(-ex0\cos\theta\sin\phi + ey0\cos\phi, -ex0\cos\theta\cos\phi - ey0\sin\phi, -ex0\sin\theta)$, and $(\sin\theta\sin\phi, \sin\theta\cos\phi, -\cos\theta)$ respectively.

inc abs1 inc1

inc_abs2 inc2

The second order absorbing boundary condition implemented allows the user to choose two angles at which the boundary condition absorbs perfectly. On the top boundary, these angles are specified by *inc1* and *inc2* (in degrees). They are measured from the z-axis.

tra abs1 tra1

tra_abs2 tra2

Similar to *inc1* and *inc2*, *tra1* and *tra2* are the perfect absorption angles at the bottom boundary in degrees measured from the z-axis.

mask mask_file

keyword mask specifies that the incident intensity is not uniform across the simulation domain. The intensity modulation information is contained in *mask_file*, a file in the PLOTMTV format which may be generated from IMAGE2D.

4.1.3 Topography

block block_num figure block_figure block_info end_block

keyword block is one of two ways to specify properties of the simulation structure. block specifies that the properties of block block_num are contained in block_info. TEMPEST continues parsing properties for block block_num until the keyword end_block is encountered. The illumination wavelength must be defined before any block information can be given. If two blocks overlap in volume, then the material properties of the overlapped

volume is determined by the latter defined block. The maximum number of blocks allowed is 120.

figure signifies that the next word defines the shape of the current block. block_figure can be one of the following:

rectangle xl xh yl yh zl zh

rectangle specifies that the current block is a rectangular box bounded in the x-direction by [xl, xh], in the y-direction by [yl, yh], and in the z-direction by [zl, zh].

sphere radius xcenter ycenter zcenter

sphere specifies that the current block is a sphere with radius radius centered at (xcenter, ycenter, zcenter).

xcylinder radius xl xh ycenter zcenter

xcylinder specifies that the current block is a circular cylinder oriented along the x-direction from xl to xh with radius radius. The circular cross-section on the yz-plane is centered at (ycenter, zcenter).

ycylinder radius yl yh zcenter xcenter

ycylinder specifies that the current block is a circular cylinder oriented along the y-direction from yl to yh with radius radius. The circular cross-section on the zx-plane is centered at (zcenter, xcenter).

zcylinder radius zl zh xcenter ycenter

zcylinder specifies that the current block is a circular cylinder oriented along the z-direction from zl to zh with radius radius. The circular cross-section on the xy-plane is centered at (xcenter, ycenter).

xwedge xl xh yl zl y2 z2 y3 z3

xwedge specifies that the current block is a wedge with a triangular interface with the yz-plane defined by the coordinates (y1, z1), (y2, z2), and (y3, z3). The wedge is oriented along the x-direction from x1 to x1.

ywedge yl yh zl xl z2 x2 z3 x3

ywedge specifies that the current block is a wedge with a triangular interface with the zx-plane defined by the coordinates (zI, xI), (z2, x2), and (z3, x3). The wedge is oriented along the y-direction from yl to yh.

zwedge zl zh xl yl x2 y2 x3 y3

zwedge specifies that the current block is a wedge with a triangular interface with the xy-plane defined by the coordinates (x1, y1), (x2, y2), and (x3, y3). The wedge is oriented along the y-direction from zl to zh.

block_info consists of a list of numbers and words, which may be:

index real_index imag_index

real_index and imag_index are respectively the real and imaginary parts of the refractive index of the current block of material. imag_index must be either greater than zero (representing dielectric loss) or equal to zero (lossless dielectric). If the value of imag_index is greater than that of real_index, "dispersive" must be specified in the input file.

eps real_eps imag_eps

real_eps and imag_eps are respectively the real and imaginary parts of the relative permittivity of the current block of material. imag_eps must be greater than zero (representing dielectric loss) or equal to zero (lossless dielectric). For each block, either index or eps, but not both, should be specified.

cond conductivity

if the current block is a metal, the properties can be specified by its conductivity conductivity. If only cond is specified, the real part of the relative permittivity is assumed to be 1.0 and the imaginary part is calculated from the value of conductivity. If both cond and eps are specified, the real part of the dielectric constant is given by real_eps, and the imaginary part is given by the sum of contributions from imag_eps and conductivity. For any block, index and cond cannot both be specified.

resist conc a b c dose step

resist specifies that the current block has dynamic change with respect to exposure. conc is the initial PAC value of the photoresist block. a is Dill's bleachable absorption coefficient of the photoresist in per micro-meter. b is Dill's unbleachable absorption coefficient of the photoresist in per micro-meter. c is the bleach rate of the photoresist model proposed by Dill in centi-meter squared per milli-Joule. dose is the total exposure energy of the photoresist in milli-Joule per centi-meter squared. The total dose is divided into step number of smaller doses, the sum of which equals the total dose. For each dose step, the steady-state electric field is computed and the bleaching of the photoresist block is modeled using Dill's ABC parameters.

read_index index_file

Another way to specify the properties of the simulation structure is by the keyword **read_index**. This loads the real and imaginary parts of the refractive index at every simulation node position from the file *index_file*. The *index_file* is consisted entirely of pairs of numbers. The number of pairs must be identical to the product of x_simulation_nodes, y_simulation_nodes and z_simulation_nodes. The first number of each pair is the real part of the refractive index and the second number is the imaginary part. The order of

the pairs is such that the first pair corresponds to the lower left corner of the simulation domain. Ordering is done by first incrementing along the x-direction, followed by the y-direction, and lastly the z-direction. A file of such format can be generated using the keyword write_index.

write_index index_file

keyword write_index specifies that the real and imaginary parts of the refractive index at every simulation node position to be written to the file index_file. This file can be used as the argument of read_index for other TEMPEST simulations.

dispersive

if the structure contains highly dispersive materials, i.e., $n_i > n_r$, the conventional algorithm is unstable. A special routine must be used by specifying **dispersive** in the input file.

4.1.4 Analysis

reflected

keyword **reflected** specifies that the reflected diffraction harmonics are calculated. The diffraction harmonics are computed at discrete scattering angles which depend on the incident wavelength and the dimensions of the simulation domain. These diffraction harmonics can be used by the post-processor IMAGE2D to generate an optical image profile of the simulated structure.

transmitted

keyword transmitted specifies that the transmitted diffraction harmonics are calculated.

no de

keyword **no_de** specifies that no diffraction harmonics are calculated. This is the default.

min_cycle min_wave_cycles

Since checking for steady-state slows down the simulation, TEMPEST excites the simulation domain min_wave_cycles wave cycles before checking for steady-state. Typically, at least 20 wave cycles of excitation are required before steady-state is reached. The number of wave cycles needed increases with complexity of the topography as well as the z_length of the simulation domain. If unspecified, the program calculates min_wave_cycles automatically.

max_cycle max_wave_cycles

Simulation continues until steady-state is reached or until the domain has been excited with *max_wave_cycles* wave cycles, whichever comes first. If steady-state is not reached before *max_wave_cycles* wave cycles of excitation, diffraction efficiencies are not calculated. A typical value for *max_wave_cycles* is 100.

err_tol fraction

Steady-state is determined by comparing the field values across an xy-plane (set at 5 simulation nodes from the boundary where the diffraction harmonics are taken, if **no_de** is specified, the plane is set at 5 simulation nodes from the top boundary) at the same instant in successive wave cycles. If the variation of the electric field at each node on the plane is less than *fraction* times a comparing value (this comparing value is determined by the specification or no specification of the keyword **err_rel**) for three consecutive wave cycles, steady-state is reached. A typical value for *fraction* is 0.02, where:

error = fraction x amplitude $|E_{new} - E_{old}| >= error$

_

err_rel

err_rel specifies that the comparing value is the instantaneous field value. If err_rel is not specified, the incident field amplitude is used as the comparing value.

4.1.5 Data

plot plot_var plot_type [fraction] [plot_dir] coor [min1 max1 min2 max2 min3
max3] plot_file

plot_var must be one of the six keywords: pac, refractive, steady, nonsteady, or transient.

pac requests a PAC concentration plot after the photoresist is exposed.

refractive requests a plot of the real part of the refractive index. This is a check to ensure that the structure is loaded into TEMPEST correctly.

steady requests a plot of the instantaneous values of a field component at steady-state. The field component is specified by *plot_dir* and the instant of the wave cycle is specified by *fraction*.

nonsteady requests a plot of the instantaneous values of a field component before the field reaches steady-state. The field component is specified by *plot_dir*, and *fraction* specifies the number of cycles after the initial excitation at which the field values are taken. Note that *instant* in this case must be smaller than *min_wave_cycles* specified in **min_cycle**.

transient requests a transient plot of a field component specified by *plot_dir*. This option traces the time development of the field value of a point in the simulation domain. When **transient** is specified, *plot_type* must be **point**.

plot_type must be one of the six keywords: point, xline, yline, zline, xyplane, yzplane, or zxplane.

point requests a plot of *plot_var* at a point in the simulation domain. This *plot_type* is usually used when a **transient** plot is requested.

xline requests a line plot of plot_var at a cutline in the x-direction from min1 to max1 at the position y=min2 and z=min3. max2 and max3 are not specified in this case.

yline requests a line plot of *plot_var* at a cutline in the y-direction from *min1* to *max1* at the position z=*min2* and x=*min3*. *max2* and *max3* are not specified in this case.

zline requests a line plot of *plot_var* at a cutline in the z-direction from *min1* to *max1* at the position x=*min2* and y=*min3*. *max2* and *max3* are not specified in this case.

xyplane requests a two-dimensional plot of $plot_var$ across an xyplane bounded by $x=\{min1,max1\}$ and $y=\{min2,max2\}$ at the position z=min3. max3 is not specified in this case.

yzplane requests a two-dimensional plot of $plot_var$ across an yzplane bounded by $y=\{min1,max1\}$ and $z=\{min2,max2\}$ at the position x=min3. max3 is not specified in this case.

zxplane requests a two-dimensional plot of $plot_var$ across an zxplane bounded by $z=\{min1,max1\}$ and $x=\{min2,max2\}$ at the position y=min3. max3 is not specified in this case.

fraction is specified only if a **steady** or **nonsteady** plot is desired. If a **steady** plot is desired, fraction is a number between 0.0 and 1.0 specifying the fraction of the wave cycle at which the plot is generated. A value of 0.0 means the beginning of a wave cycle and a value of 0.25 means a quarter of a wave cycle after the beginning (a phase of 90 degrees). If a **nonsteady** plot is desired, a plot after fraction cycles of excitation is generated. Note that for a **nonsteady** plot, the value of fraction must be a number between 0.0 and min_wave_cycles.

plot_dir is specified only if plot_var is one of steady, nonsteady, or transient. plot_dir contains two entries. The first entry is either e, h, or s, specifying the electric field, the magnetic field, or the Poynting vector. The second entry can be one of the following: x, y, z, or t. x, y, or z specifies the direction of the field, and t specifies that the total field (magnitude) is requested.

coor can be either of the two keywords **position** or **node**. **position** specifies that the coordinates min1, max1, min2, max2, min3, and max3 are specified in micrometers. **node** specifies that min1, max1, min2, max2, min3, and max3 correspond to the simulation node number. The convention is that (0, 0, 0) corresponds to the spatial location (0, 0, 0) and $(x_simulation_nodes, y_simulation_nodes, z_simulation_nodes)$ corresponds to $(x_length, y_length, z_length)$.

plot_file is the name of the file to which data are written. All the data files are in the PLOTMTV format. A maximum of 50 plots can be generated.

4.2 TEMPEST commands

4.2.1 jrun

Selected sections of the manual pages of jrun are shown below. Interested users can read the on-line manual by typing

cm% man jrun

NAME

jrun - run a job interactively (DJM)

SYNOPSIS

jrun [file] [options]

jrun [options] -- file [arguments]

DESCRIPTION

The jrun command runs a job interactively. The output is directed to your terminal and the input is obtained from your keyboard. To disconnect your terminal from the job, type a tilde (~) followed by control-B (^B). After you disconnect, the input and output will be redirected to disk files or /dev/null as indicated by the -stdin and -stdout options. The job can later be reconnected to the terminal using jconnect.

If no program is specified on the command line, your login shell is invoked and an interactive login session is created. The options to **jrun** are a superset of those provided by **jsub**. Options may be specified on the command line or they can appear as embedded comment directives within the job's shell script. See **jsub**.

At minimum you must specify the following options: -nproc, -cputime, and -memory. These are required by DJM in order to schedule jobs effectively. When disconnected, output will be sent to a file with the same name as the job file with the suffix .onnn appended, where nnn is the job id. If the EMACS environment variable is set, jrun assumes it is running inside of an emacs shell-mode buffer.

OPTIONS

The options unique to **jrun** are defined below. See **jsub** for a definition of the remaining options.

-capture

Always capture output to the -stdout file, even when the job is connected to the terminal. Normally output is captured only when the job is disconnected.

-echo

Turn on echo. The session will echo characters typed at the terminal. This is the default.

-emacs

Turn on emacs mode. This option is useful when using **jrun** inside of an emacs shell-mode buffer. It disables character echo and disables control-S

and control-Q processing. This option overrides the EMACS environment variable.

-noecho

The session should not echo characters typed at the terminal.

-noemacs

Turn off emacs mode. This option overrides the EMACS environment variable.

-eightbit

Pass 8-bit characters through unchanged. By default the uppermost bit of each character is stripped off to create 7-bit logical characters.

4.2.2 jsub

Selected sections of the manual pages of **jsub** are shown below. Interested users can read the on-line manual by typing

cm% man jsub

NAME

jsub - submit a job for background execution (DJM)

SYNOPSIS

jsub [file] [options]
jsub [options] -- file arguments]

DESCRIPTION

The **jsub** command submits a file containing a program or a shell script for execution on a machine. The job will be executed in the same directory in which the job was submitted. The job will be run in the background and all output will be directed to a file. The job can be connected to a terminal if the -tty option is set. See **jconnect**.

jsub is upward compatible with the command **qsub** in the Network Queuing System (NQS).

Options may be specified on the command line or they can appear as embedded comment directives within the job's shell script. Such directives consist of a shell comment character (#) followed by a special prefix: either J, JSUB, QSUB, PBS, or @\$. The first line of the script can begin with #! to specify a shell to interpret the script. Example: #!/bin/sh. If omitted, the login shell is used.

An example is shown below of using embedded comment directives in a job script.

#!/bin/sh the name of the shell #JSUB -nproc 8K #JSUB -cpu 60min -mem 128mb #JSUB a.out # run my program Directives are evaluated up to the first non-blank, non-comment line or up to the first directive with no - present.

The output will be sent to a file with the same name as the job with the suffix .onnn appended, where nnn is the job id. By default, the standard output and the standard error are combined into a single stream and sent to this file. You can redirect the standard error to a different file with the -stderr option. This option will not work if -tty is set because there is no way to disambiguate output sent to a terminal device.

At minimum you must specify the following options: -nproc, -cputime, and -memory. These are required by DJM in order to schedule jobs effectively. It is in your best interest to estimate these resource values as accurately as possible with respect to your job's actual needs. If you understate your job's resource requirements, your job may be terminated by DJM if other jobs are waiting to run. On the other hand, you should not overestimate your resource requirements as that may cause your job's execution to be delayed. These estimates are treated as "soft" limits when your job runs. Your job is not automatically killed if they are exceeded. The chance of getting killed depends on how egregious the overrun is and how heavily loaded the machine is.

The actual resource usage is written to the end of the output when your job finishes. You can use this information to supply improved usage estimates the next time you run your job.

OPTIONS

All option names may be abbreviated to uniqueness.

-machine mach

Execute the job on machine mach. This is typically the name of a Connection Machine (Reg.) system. By default the machine name is obtained from the environment variable DJM_MACHINE.

-cputime n

Request n units of CPU time. The suffix secs indicates seconds, min indicates minutes, hr indicates hours, and days indicates days. The default is min. Suffixes may be abbreviated. Example: -cpu 10h. The amount of time is limited based on per-queue and global maximums. See jstat limits.

-memory n

Request n units of memory. The suffix kb indicates kilobytes, kw indicates kilowords (8192 bytes), mb indicates megabytes, mw indicates megawords, gb indicates gigabytes, and gw indicates gigawords. The default is megabytes. A single letter abbreviation indicates a byte (not word) unit. Example: -mem 2g. The amount of memory is limited based on per-queue and global maximums. Note that the amount represents total memory, not memory per processor.

-nproc n

Request at least n processors. The suffix k indicates 1,024 processors. Note that this represents a minimum requirement: your job may actually be run on

a partition with more processors than you requested if the partition is available. If you require exactly n processors, add the **-exact_proc** option.

-dedicate

Request dedicated access to the partition. Your job will have the right to access of all resources (memory, cpu, nproc) of the partition during its execution. The -memory option is ignored, as you own all of the memory by definition. The job will only be run when there exists a partition that is enabled for dedicated access. Typically the operator will create one such partition encompassing the entire machine overnight. Dedicated partitions have special scheduling rules. See the DJM Administration Guide for more details. (NOTE: Do not confuse -dedicated with -notimeshared. The latter merely runs a job on a sequencer that does not have a timesharing daemon.)

-after time

Defer execution of the job until after the indicated time (or date). If the parameter contains embedded spaces, it must be enclosed in quotes, for example: -after "July 14 12:30pm".

-hard_cputime n

Specify a hard limit for cpu time. If your job exceeds this limit, it is killed immediately. This is useful for preventing a runaway job from consuming all of a user's account allocation.

-help

Display a summary of all options along with a one line description of each option.

EXAMPLE

cm% cat myjob

```
#!/bin/sh
# This script shows an example of embedded DJM comment directives
#JSUB -procs 8K
#JSUB -cpu 60min
#JSUB -mem 80M
a.out
                   cm% jsub myjob -mach cm200
                   Job submitted successfully. Job id is 57.
                   (one hour later)
                   cm% cat myjob.o57
*** Distributed Job Manager 1.0, CM-200 (pa) AHPCRC / Minn. Supercomputer Ctr
*** job57 procs 8192, mem 80M, cpu 60min, seq 2, server cb:0
*** alan /bin/sh myjob started on Fri May 22 14:18:01 1992
Attached to {CM}* timesharing on CM-MSC, a CM200 on interface 0
Attached to 8192 CM200 processors on sequencer 2, microcode version 6104
1024K of memory with 64 bit floating point. Paris safety is on.
+ a.out
Working...
```

```
I'm done.

Detached from (CM)* Timesharing.

*** Job terminated at Fri May 22 15:20:15 1992

*** exitcode = 0000

*** procs 8192, mem 43M, cpu 52min

***

*** You requested 80M of memory but only used 43M.

*** The next time you run this job, you should request

*** less memory. This will let your job run earlier

*** and you will get your results sooner.
```

NOTES

There are per-queue and per-user limits on the number of jobs that can be submitted at the same time.

A jsub job with the -tty option is indistinguishable from a jrun job. The Posix Batch System (IEEE Std 1003.15) changed the way options are parsed, requiring all options to consist of a single letter. DJM, on the other hand, has many more arguments than available letters in the alphabet. This means that options which can be grouped together in PBS (for example, -zV) must be broken apart in DJM (-z -V).

4.2.3 TEMPEST

The program TEMPEST takes two arguments. The first of which is the name of the input file which contains the topography information. The second argument is the name of the output file to which information on the diffraction harmonics is written.

cm% tempest input_file output_file

4.3 Pre-TEMPEST Workstation Commands

4.3.1 CHECK

Since computation time on the CM is expensive, it is desirable to ensure that the format of the input file is correct before submitting the input file for simulation. The CHECK routine checks for possible errors in the input file. The program CHECK is invoked in the following way:

ws% check input_file

where *input_file* is the input file to TEMPEST. If the input file *input_file* contains mistakes such as incorrect keywords, CHECK notifies the user of the mistake.

4.4 Post-TEMPEST Workstation Commands

4.4.1 **IMAGE2D**

Based on the information of the diffraction harmonics contained in the output file, the optical image profile of the simulated structure can be synthesized given the characteristics of the optical system including the numerical aperture (NA), partial coherence factor (σ), and the magnification factor. This is done by the program IMAGE2D, which calls SPLAT to calculate the aerial images. Since TEMPEST assumes coherent illumination, partial coherence in the IMAGE routine is modeled by Hopkins' approach¹. Two assumptions are made:

- 1. The magnitudes of the diffraction efficiencies are independent of the angle of illumination.
- 2. The illumination energy is distributed evenly over the illumination cone.

With these assumptions, the intensity at every point in space can be calculated by evaluating the transmission cross coefficients¹. This approach can be used to model bright-field or dark-field optical systems, arbitrary lens aberrations as well as defocus effects.

IMAGE2D is invoked with the following command:

image TEMPEST_output_file [-na NA] [-sg sigma] [-f defocus] [-m magnification] [-x x_displace] [-y y_displace] [-t x_pts y_pts] [-p]

TEMPEST_output_file is any output file generated from TEMPEST which contains information on the diffraction efficiencies. Optical image profiles at the defocus level specified by defocus is calculated and displayed on the screen if the [-p] flag is specified. The image data is written to the file TEM-PEST_output_file.mtv in PLOTMTV format. If the user is working on a terminal with no graphical facility, the [-p] flag should not be specified. The characteristics of the optical system are described by the flags [-na], [-sg], and [-m]. NA is the numerical aperture of the optical system; sigma is the partial coherence factor of the system; magnification is the magnification factor.

Based on the parameters specified on the input line, IMAGE2D creates a SPLAT input file called *TEMPEST_output_file.spl*. The user can modify this SPLAT input file to model different optical system characteristics such as modified illumination, pupil filtering, lens aberrations, and/or thin-film effects. Please refer to the SPLAT Users' Guide³ for more information.

-na NA

numerical aperture of the optical system. The default is 0.5

-sg sigma

sigma is the partial coherence factor. The default is 0.5

-f defocus

defocus is the amount of defocus in micro-meter. The default is 0.0

-m magnification

magnification is the magnification factor of the mask. For example, -m 4 means that it is a 4X reduction system. The default is 5.

-x x_displace

displaces the calculated image by $x_displace \mu m$ in the x-direction. The option is used to facilitate the displaying of the image.

-y y_displace

displaces the calculated image by $y_displace \mu m$ in the y-direction. The option is used to facilitate the displaying of the image.

-t x_pts y_pts

the optical image data is written to the file $TEMPEST_output_file.mtv$ with x_pts data points in the x-direction and y_pts data points in the y-direction.

-p

displays the calculated image on the terminal.

4.4.2 PLOTMTV

PLOTMTV is developed by Kenny Toh at Intel Corporation. It is available in the public domain and is distributed along with TEMPEST. Files in the PLOTMTV format can be plotted using the command:

ws% plotmtv [-nodate] [-colorps] [-l] file_name

where file_name is the name of the data file. If [-nodate] is specified, the postscript file generated by PLOTMTV has not date stamp on it. To generate color postscript files, specify the [-colorps] option. The [-l] option specifies that the graph is plotted in the landscape orientation.

4.4.3 AMPHA1D and AMPHA2D

The amplitudes and phases of the electromagnetic can be calculated from the instantaneous field values using the routines AMPHA1D and AMPHA2D. These two routines take as input two data files corresponding to the instantaneously field values at two instants separated by a quarter of a wave cycle. Two data files are generated which contain respectively the amplitude and phase information.

The synopses of amphald and ampha2d are identical. For one-dimensional data files (i.e., data files generated with *plot_type* equal to xline, yline, or zline), amphald is used. For two-dimensional data files (i.e., data files generated with *plot_type* equal to xyplane, yzplane, or zxplane), ampha2d is used.

ws% ampha1d/2d file_000 file_250 file_amp file_pha

where file_000 and file_250 are the input data files. file_250 contains field values which occur a quarter of a wave cycle later than the data in file_000. file_amp and file_pha contain the amplitude and phase information respectively. The data files file_000 and file_250 can be generated using the TEMPEST input keyword plot as described in Section 4.1.5. For an example, please refer to the TEMPEST input file shown in Section 3.2.

4.4.4 FACTOR1D and FACTOR2D

In some cases the user may wish to scale an axis of a plot file in the PLOTMTV format. For example, the user may wish to normalize the optical image profile to a certain level. This is accomplished by the routines FACTOR1D and FACTOR2D.

For line plots, use

ws% factor1d input_file output_file dir factor

where *input_file* is the data file in PLOTMTV format and *output_file* is the name of the file to which the modified data is written. *dir* is either x or y, specifying either the x-axis or the y-axis is scaled by a factor of *factor*.

For two-dimensional plots, use

ws% factor2d input_file output_file factor

where *input_file* is the data file in PLOTMTV format and *output_file* contains the modified data. All the data points are multiplied by a factor of *factor*.

4.4.5 REDUCE2D

Sometimes the size of the data file is so large that processing is extremely slow and takes up too much disk space. One way to speed up processing and reduce storage memory is by reducing the number of data points with the routine **reduce2d** as follows:

ws% reduce2d input_file output_file x_factor y_factor

In the x-direction, reduce2d takes one datum out of every x_factor data from input_file. In the y-direction, the program takes one datum out of every y_factor data from input_file. The reduced data set is written to output_file. The size of output_file is thus $(x_factor^*y_factor)$ times smaller than input_file. From experience, taking one datum out of two to four data from a raw TEMPEST data file retains the resolution yet improves processing time and reduces storage memory.

Useful Hints Useful Hints 5.1 Top and Bottom of the Simulated Structure The materials at the top and bottom of the simulated domain must be homogeneous. Also, the entire simulation domain must be filled (material properties specified). It is suggested that the first block of material is defined to be a rectangular box with dimensions conforming to the size of the simulation domain. 5.2 Material Interface from the Top and Bottom Boundaries If a material interface exists very close to the top of the simulation domain, simulation results may be inaccurate. The distance between an interface and the top of the simulation domain should be about one wavelength. This consideration applies to the interface closest to the bottom of the simulation domain as well. Also, material properties must be uniform across the top and bottom boundaries of the simulation domain. 5.3 Verification of Loaded Topography If it is suspected that the loaded topography does not coincide with which the user has in mind, the user can verify the loaded topography by plotting the real part of the refractive index using the keyword **plot** as described in Section 4.1.5. 5.4 Real and Imaginary Parts of the Refractive Index Numerical instability may occur when the imaginary part of the refractive index of a particular material block is greater than the real part. Such a situation may arise if a metal block is present. In such instances, the line "dispersive" must be included in the input file to TEMPEST.

5.5 Number of Simulation Nodes

The number of simulation nodes needed in order to give accurate simulation results can be determined by the following relation:

 $x_simulation_nodes > (15*largest_index*x_length)/wavelength$

and the number of simulation nodes in the y- and z-directions can be determined from x_simulation_nodes by the ratios of x_length, y_length and z_length.

	Useful Hints
5.6	Periodic and Isolated Structures
	In the current version, isolated structures cannot be analyzed. periodic structures must be assumed. Isolated structures can be modeled by using a large periodic simulation domain.
5.7	Convergence Problems

If the user encounters convergence problems (which should not be any), try adding the line " $dtfrac\ 0.5$ " to the TEMPEST input file.

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Appendix A Summary of Commands

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Appendix B Connection Machine Facilities

The following list of connection machine facilities was obtained from David Ray (ray@think.com) of the Customer Support Group, Thinking Machines Corporation.

B.1 Thinking Machines Corporation - Connection Machine Network Server (CMNS) Pilot Facility

Address: CMNS Facilities Manager

Thinking Machines Corp.

245 First Street

Cambridge, MA 02142-1214

Phone:

(617)876-1111 ext. 2121

Electronic Mail:cmns-manager@think.com

ames!think!cmns.manager uucp:

B.2 NASA Ames Research Center

Address: Mail Stop T045-1

Moffett Field, CA 94035

Phone: Bruce Blaylock (415)604-4400

Dave Gambrel (415)604-4504

B.3 National Center for Supercomputing Applications (NCSA)

Address: Metacomputer Allocations

National Center for Supercomputing Applications

257 Computing Applications Building

605 E. Springfield Ave.

Champaign, IL 61820

Contact: allocations

(217)244-0635

allocations@ncsa.uiuc.edu

B.4 Northeast Parallel Architectures Center (NPAC)

Address: NPAC - Syracuse University

111 College Place

Science & Technology Bldg.

Machine Room 1-213 Syracuse, NY 13244-1240

Phone:

(315)443-1722

Fax:

(315)443-1973

Contact: Don Hewitt

(315)443-2086

don@nova.npac.syr.edu

Connection Machine Facilities

B.5 Naval Research Laboratory (NRL) [Code 51-30]

Address: 4555 Overlook Ave., SW

Washington, DC 20375-5000

Phone: (202)404-7020 or (202)404-7029

Contacts: Henry Dardy (202)404-7028 dardy@cmvax.nrl.navy.mil

CM-Room (202)767-9044 or (202)767-9045