

Application of Multifrontal Method for Doubly-Bordered Sparse Matrix in Laser Diode Simulator

Y.S. Chen* and Z. Simon Li**

*Crosslight Software Shanghai Branch, China, email: cys@crosslight.com.cn

**Crosslight Software Inc., Burnaby, Canada, email: simon@crosslight.com

Linear systems in a laser diode simulator such as LASTIP[1] are typically sparse, asymmetric and poorly scaled. Its factorization is a computation bottleneck in numerical simulation. The multifrontal (MF) method is robust and efficient for large sparse nonsymmetrical matrices and it has become more important as laser diode structure design becomes more sophisticated with increasing matrix size.

A unique pattern of the sparse matrix of LASTIP comes from the discretization of the following photon rate equation.

$$v_g(g_m - \alpha_{int} - \alpha_{em})S + c_m \int R_{sp} dx dy = \partial S / \partial t$$

The first three terms are modal gain, internal loss and mirror loss. The last term on the left hand side is the spontaneous recombination rate averaged over the whole device. The most important term of integration comes from the modal gain which can be expressed in terms of the local gain integrated over the whole device. S is the linear photon density for a particular lateral mode and is treated as an independent variable to be solved by the Newton solver. There are as many such integral equations as the number of lateral modes. When these integral equations are ordered towards the end of the usual nodal discretization of the drift-diffusion equations, a doubly-bordered matrix pattern is formed with the width of the border equal to the number of lateral modes (see Fig. 1).

The classical multifrontal method assumes structural symmetry. For asymmetric matrix A, we use $A + A^T$ to store explicit zeros. The symmetry of a typical matrix from LASTIP is around 0.8 which is close to unity. So we can use the structural symmetry pattern in the symbolic analyze. The asymmetric frontals are used in the numeric factorization[2] to reduce fill-in.

The border percentage (the percentage of non-zero entries in the border among all non-zeros) of the typical matrices is from 20%~50%, which can be used by block algorithm as follows. Suppose A is the doubly-bordered matrix, we write

$$A = \begin{bmatrix} B & C \\ R & D \end{bmatrix} = \begin{bmatrix} L' & \\ R' & D_L \end{bmatrix} \begin{bmatrix} U' & C' \\ & D_U \end{bmatrix}$$

where C is dense columns, R is dense rows. B is a sparse block which can be factored as $L'U'$ by the classical multifrontal method.

$$R' = RU'^{-1}, C' = L'^{-1}C, D - R'C' = D_L D_U.$$

The advantages for the above algorithm is as follows: 1) Less time and

storage space in symbolic analyze; 2) Less storage allocation and data movement during numeric factorization; 3) More convenient for parallel computation when treating doubly-bordered structure [3]. Work is underway to verify 3) for parallel computation.

Table 1. lists the example name, mesh points and the border percentage of 6 examples from LASTIP. The last two columns are the run times of the old vectorized sparse solver and the multifrontal solver. The largest speed up is more than 6 times with 7938 mesh point and mode_num=6,. Figure 1 is the matrix pattern showing the double border. Figure 2 is the mesh and figure 3 is wave intensity indicating the coverage of the wave intensity over the whole device.

In conclusion, we find that the MF method can be applied to doubly-bordered sparse matrices arising from laser diode simulators with substantial increase in speed especially for larger matrix size.

[1] Lastip User's Manual. Crosslight Software. Version 2003.12

[2] PR Amestoy and C. Puglisi, An unsymmetrized multifrontal LU factorization, Technical report ENSEEIHT-IRIT RT/APO/00/3 .

[3] Tariq Rashid, Timothy A. Davis: An Approach for Parallelizing any General Unsymmetric Sparse Matrix Algorithm. PPSC 1995: 413-417

Table 1: Run time in seconds

name	mesh	BLU%	old	MF
beamst	648	36	19.1	15
bulk2dmul	1026	21.5	29.9	21.7
gaas20	592	0	11.7	7.9
gaas26	7938	44	1705.8	277.8
ox	736	58.2	27	16.5
q_ridge	3420	36	234.7	107.1

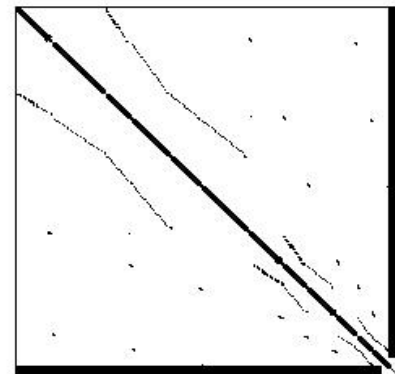


Figure 1 Pattern of gaas26

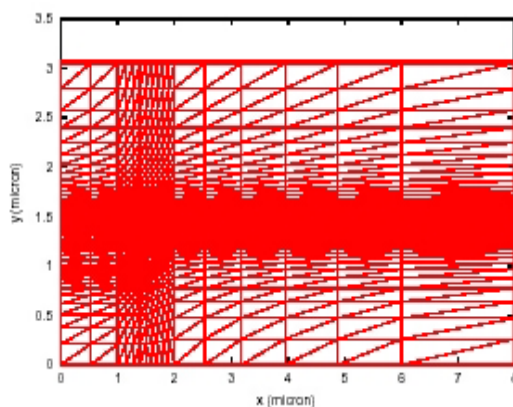


Figure 2. Mesh of gaas26 structure

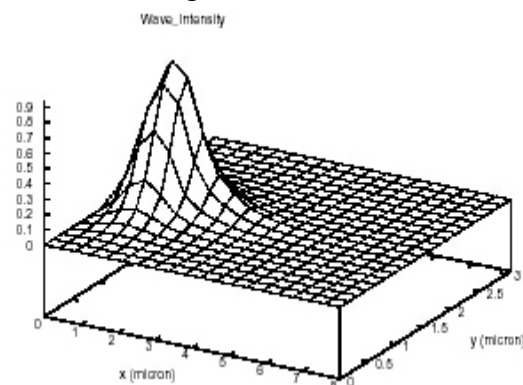


Figure 3. Wave of the 2nd mode