High Performance Scientific Computing (3-1-0-0)

Objective:

Discussing storage and solution techniques for large matrices arising from physical and engineering system analysis. Exploring techniques for faster convergence. Understanding basics of parallel computing. Hands on MPI, OpenMP and CUDA. Applying MPI and CUDA for efficient solution of large matrices.

Students are expected to have preliminary background in linear algebra and computer programming (C/Fortran)

Contents and Lecture Hours:

Topics	**Hours (L-T)**
Sparse Matrices Discretization of differential equations, Storage Schemes for sparse matrices, Permutations and reorderings, Direct Solution Methods	**6L,2T**
Iterative methods and Convergence SOR, Gradient search Methods: steepest descent, Conjugate gradient algorithm, Krylov subspaces methods: Arnoldi's method, GMRES, Symmetric Lanczos algorithm, Convergence Analysis, Block Krylov Methods, Preconditioning techniques, ILU factorization preconditioners, Multigrid methods.	**11L,4T**
Domain Decomposition Schwarz algorithms and the Schur Complement Graph partitioning: Geometric Approach, Spectral Techniques	**4L, 1T**
Parallel Computing Architectures for parallel computing, Shared and distributed memory Performance metrics, Parallelization of simple algorithms	**4L**

MPI and OpenMP Basic MPI and OpenMP calls Parallelizing matrix solvers using domain decomposition	**8L,4T**
CUDA GPGPU architecture Thread algebra for Matrix operations Accelerating Matrix solvers using CUDA	**7L,3T**

Books:

1. Yousef Saad, Iterative Methods for Sparse Linear Systems, SIAM 2003.

2. G H Golub and C F Van Loan, Matrix Computations, The John Hopkins University Press.

3. A Grama, A Gupta, G Karypis and V Kumar, Introduction to Parallel Computing, Addison Wesley

4. Gropp, William, Ewing Lusk, and Anthony Skjellum. Using MPI: portable parallel programming with the message-passing interface. Vol. 1. MIT press, 1999.

5. Shane Cook, CUDA Programming: A Developer's Guide to Parallel Computing with GPUs, M K Publishers

6. Journal of Computational Physics, Journal of Supercomputing