

COMP 705: Advanced Parallel Computing

HW 6: Accessing XSEDE resources; parallel NetCDF

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Problem 6a: Accessing comet.sdsc.edu

- Use your parallel MPI I/O (or NetCDF) code to show you can access and run jobs on comet.
- This includes:
 - Logging on
 - Setting your environment
 - Running batch script jobs

Problem 6b: Using Parallel NetCDF Data Storage

- Note: this problem is no longer required for HW4 (running on tuckoo)
- Modify your code to save temperature data at different time slices into a single NetCDF file
- You will need to define your own meta data and arrays to store. Examples include:
 - data stored in structs, temperature, time data
 - create names for data, and scalings (min/max temp, min/max temperature, etc.)
- Visualize 3 or more timeslices using software that can read your netCDF file.

HW 6 Instructions

- For this HW, you will work with your 2D Iterative solver to modernize and optimize the code.
- Code features will include:
 - Dynamic/command line arg processing for both processor and problem distributions.
 - Using 1D communicator groups for subarray data exchange
 - Use of MPI datatypes, including MPI_Type_structs, MPI_Type_vector, and MPI_Type_create_subarray
- You will use different MPI_File I/O and netCDF protocols to store your data.

Configuration for all Problems

- Modify code to process command line arguments for PE's and ProbSize
- Define an MPI_Type_structs to hold configuration information for each node.
- Types of structs & data would include:
 - distribution: rank, problem size,
 - grid: problem size, start and end index
 - time: total time, number of measurements
- consider a local and global data structure.

Configuring the Problem Size and Processor Distribution

- 2D block-block data distribution: $M(n_i, n_j)$
 - where the range of $n_i = [1 : M_{Imax}]$;
 - where the range of $n_j = [1 : M_{Jmax}]$;
 - $sizeof(M) = n_i * n_j$
 - set default to be $n_i = n_j$
- 2D cartesian processor arrangement: $P(p_i, p_j)$
 - where the range of $p_i = [1 : P_{Imax}]$;
 - where the range of $p_j = [1 : P_{Jmax}]$;
 - $NP = p_i * p_j * p_k$
 - set default to be $p_i = p_j$
- Save as MPI struct datatypes; use to communicate to other cores

Analysis

- Compare serial to parallel as a function of PE configurations, problem sizes, and File I/O mechanisms.
- Plot speedup
- Use TAU/ParaProf to identify bottlenecks; you can include images to show what you did.
- See notes at:
<https://edoras.sdsu.edu/~mthomas/f17.705/topics/perf//>

TAU: Using ParaProf to visualize profile files.

TAU: ParaProf: Function Data Window: /home/mthomas/pardev/matmul/mpi/wa...

File Options Windows Help

Name: Local_matrix_multiply [{/home/mthomas/pardev/matmul/mpi/wave-mpt/wave-dyn-mpt.c}
{919,0}]

Metric Name: TIME

Value: Exclusive

Units: seconds



Matlab code to read NetCDF Data (pg 1/3)

```
% pres_temp_4D matlab code
% Created by Mary Thomas San Diego State University
% Matlab code based on tutorial at:
% http://www.public.asu.edu/~hhuang38/matlab-netcdf-guide.pdf
%
clear all;
%%
home='/netcdf/ser/simple ';
ncfile=[home,'/','pres_temp_4D.nc'];
fprintf('Analyzing data file: %s \n', ncfile);

%% netCDF has 3 header sections:  dimensions; variables; data
% dump the data to stdio
ncdisp ( 'pres_temp_4D.nc' );

%% Step 1: Open the file
ncid1 = netcdf.open(ncfile,'NC_NOWRITE');
fprintf('netCDF data file has been opened. \n');

%% Steps 2—4 are often not necessary if one has already obtained
% the needed information about specific variables by running ncdisp in Step 0.

%% Step 2: Inspect the number of variables and number of dimensions, etc., in the file
fprintf(' \n');
[ndim, nvar, natt, unlim] = netcdf.inq(ncid1);
fprintf('netCDF file insp: ndims=%d], nvars=%d], natt=%d], unlim=%d] \n', ...
        ndim, nvar, natt, unlim);
fprintf(' \n');

%% Step 3: Extract further information for each "dimension"
for i=0:ndim-1
    [dimname, dimlength] = netcdf.inqDim(ncid1, i);
    fprintf('netcdf.inqDim[%d]: dimname=%s], dimlength[%d] \n',i, dimname, dimlength);
end
fprintf(' \n');
```

Matlab code to read NetCDF Data (pg 2/2)

```

%% Step 4: Extract further information for each variable
for i=0:nvar-1
    [varname, xtype, dimid, natt] = netcdf.inqVar(ncid1, i);
    %dimid
    fprintf('netcdf.inqVar[%d]: varname=%s, xtype=%f, natt=%d\n', i, varname, xtype, natt);
end
fprintf(' \n');

%%% read var 1 == latitude
lat1 = netcdf.getVar(ncid1,0,0,6);
lon1 = netcdf.getVar(ncid1,1,0,12);
[n,lev1] = netcdf.inqDim(ncid1, 0);
%%% pres_out[nlat][nlon]
% #define NLVL 2
% #define NLAT 6
% #define NLON 12
%
% = netcdf.getVar(ncid1, varid, start, count)
fprintf('Setting up to read pressure data \n');
pres_varid=2;

% this is a 4D variable
pressure = netcdf.getVar(ncid1, pres_varid);

%message/extract 2D data
for p = 1:12 %lon
    for q = 1:6 %lat
        map1(q,p) = double(pressure(p,q));
    end
end
end

```

Matlab code to read NetCDF Data (pg 3/3)

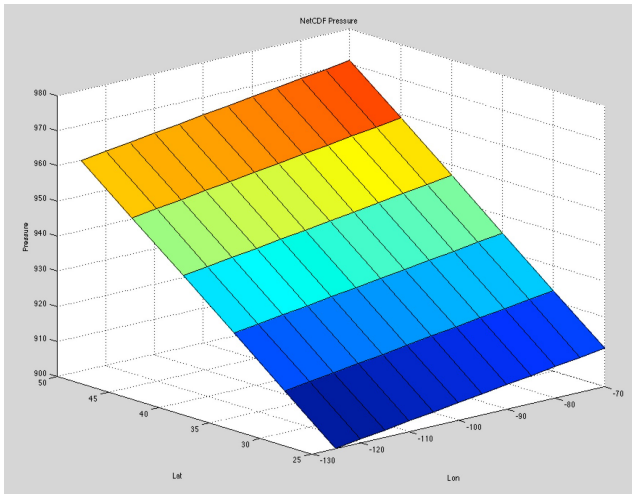
```
% Plot the mapped data
pcolor(lon1,lat1,map1);
shading interp
colorbar
hold on
contour(lon1,lat1,map1,'k-')

grid on;

break;

%%
surface(lon1,lat1,map1);
xlabel('Lon');
ylabel('Lat');
zlabel('Pressure ');
title('NetCDF Pressure ');
grid on;
```

TAU: Using ParaProf to visualize profile files.



Simple plot of pressure data from netCDF file.