Profiling of the operational and experimental code of the National Air Quality Forecasting Capability (12km horizontal grid spacing) running on NCEP’s p6 Supercomputer

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INTRODUCTION

Table 1. CMAQ configurations

<table>
<thead>
<tr>
<th>Run slot</th>
<th>Gas-chemistry mechanism</th>
<th>Aerosol module</th>
</tr>
</thead>
<tbody>
<tr>
<td>Production</td>
<td>CBM-IV aero3</td>
<td></td>
</tr>
<tr>
<td>Experimental</td>
<td>CBO5</td>
<td>aer04</td>
</tr>
</tbody>
</table>

The benefit of speedup due to extending the forecasting time and geographical coverage, finer horizontal and vertical grid spacing, optimizing NAQFC with respect to the operational machine is important. Last fall, NCEP had upgraded its supercomputer to IBM’s p6 hardware (see Fig. 1). Profiling of CMAQ with configurations shown in Table 1, on this new machine aims to better optimize the code by addressing:

- diminishing speedup with respect to increasing resource allocation;
- refine granularity analysis for I/O and communication overheads for the science processes.

The huge disparity in utilization rates between the minimum and maximum values stems from the disparity of cloudsiness, chemical regimes, and PBL structure attributing to the intrinsically uneven balanced problem in parallelizing "cldp", "chem", and "vdif", respectively.

SUMMARY

The master PE is the dedicated “output” PE. It was not a major factor in holding up wall-clock time as shown in Table 3. Most of its time is spent waiting for the slave PE’s to deliver results.

Miscellaneous Code Segments (computational details)

- Subroutine DETPRC: aerosol density, Cg, etc
- Subroutine ORGAERO for SOA
- Subroutine PCCPC for heterogeneous NOx reaction
- Moments, number-concentration and partition calculation, mean free path, and aerosol mass
- Size-dependent condensation growth factors for sulfate and organics
- New particle due to binary nucleation of H2SO4 and H2O
- Coagulation (analytical) within and between modes
- Update number concentration of Aitken (Riccati Eq.)
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