Atmospheric Composition Change and Its Climate Impact Studied by Global and Regional Chemical Transport Models

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The FRSGC/UCI Global Chemical Transport Model has been successfully ported to the Earth Simulator, and parallelization is currently under way. The CTM is run at T63 (1.9 degree) resolution with 40 vertical levels; this matches the highest resolution that global models treating tropospheric chemistry have been run anywhere in the world. The CTM has previously been run on NEC SX5 machines in single-processor mode, and is heavily optimized for vector operation on these machines. Work this year focused on porting the code to the Earth Simulator, rerunning previous simulations to verify that changes were correctly implemented, and assessing appropriate methods for parallelization.

Tthe ES-adapted global atmospheric tracer transport model, optimized for transporting large number of inert/slowly reacting tracers for inverse model studies has been completed. The model demonstrated to run in parallel on up to 10 nodes and 80 processors. No performance degradation with increase of the number of nodes is observed, because all tasks including preprocessing are done in previous version on each processor.

Keywords: Chemical Transport Model, Atmospheric Transport Model, Chemical Processing, Inverse Modeling

Results

1. Detailed Purpose of the Project

High resolution analysis of the Asian regional atmospheric chemistry and composition, its relation with industrial and natural sources in the area. Establish high resolution global atmospheric chemistry modeling, analyze intercontinental transport of pollution and its impact on regional chemistry. Improve the understanding of the spatial and temporal variability in global carbon cycle through development and application of the next generation inverse models based on atmospheric CO_2 observations and atmospheric transport models.

2. Brief Description of Simulation Programs

Parallel regional atmospheric chemistry simulation and real-time forecast system (I. Uno, Z. Wang). Online tracer transport in the mesoscale atmospheric model with detailed atmospheric chemistry mechanism.

Global atmospheric chemistry model (M.Prather, O.Wild). Global offline tracer transport with ECMWF winds and fluxes at T63 res. Detailed atmospheric photochemistry, 2nd moment conserving transport algorithm (M.Prather)

Global tracer transport model with offline winds, setup optimized for inverse modeling of surface fluxes. Transport model optimized to transport multiple signals in parallel.

3. Annual Schedule

Conduct simulations of the temporal variability in the global carbon cycle using high-resolution atmospheric transport and inverse models. Use inverse models for observation systems design and assessment.

Long Term. FY 2004-2005

Continue research on the global analysis using high-resolution transport, inversion and high resolution models of terrestrial and oceanic fluxes of CO_2 and other GHG

4. Attained Result by Using the Earth Simulator in FY 2002

4.1. The FRSGC/UCI Global Chemical Transport Model

The FRSGC/UCI Global Chemical Transport Model has been successfully ported to the Earth Simulator, and parallelization is currently under way. The CTM is run at T63 (1.9 degree) resolution with 40 vertical levels; this matches the highest resolution that global models treating tropospheric chemistry have been run anywhere in the world. Once the CTM has been fully optimized for the Earth Simulator, it is hoped to run at T106 (1.1 degree) resolution, taking it into a leading position for research into the processes affecting tropospheric composition. High resolution is important not just for capturing dynamical features associated with meteorology, but for resolving non linearities in chemical processing. Production of ozone, a major pollutant and an important greenhouse gas, is dependent on emitted precursors in a strongly non-linear way, and there are currently significant differences in ozone production between simulations conducted in high-resolution regional models and those in the lower-resolution global models that are required to assess its global impacts. Higher resolution global models will be able to address these processes more accurately.

The CTM has previously been run on NEC SX5 machines in single-processor mode, and is heavily optimized for vector operation on these machines. Work this year focused on porting the code to the Earth Simulator, rerunning previous simulations to verify that changes were correctly implemented, and assessing appropriate methods for parallelization. To verify the suitability of the code for parallelization without substantial rearrangements, we initially implemented OpenMP to run the code on 8 processors on a single node from shared memory. This provided substantial performance enhancements, while clarifying which algorithms used in the code will need further optimization. Work is now planned to alter the code structure to make use of multiple nodes using MPI. While the scalability of the code is good for dynamics and for chemical algorithms, a number of bottlenecks remain, principally in diagnostic code and in the sections of the code requiring large quantities of input data. Future optimization will focus on these sections.

4.2. Completed development of the ES-adapted global atmospheric tracer transport model, optimized for transporting large number of inert/slowly reacting tracers for inverse model studies.

Global distribution of the greenhouse gas fluxes are obtained by first calculating source-receptor matrixes with forward transport model and then applying an inverse model to fit model fluxes to the observations. This approach is severely constrained by existing capabilities of global transport simulation of multiple tracers.

In this application, independent transport simulation of different non-reacting tracers is possible, and can be done in parallel running different tracers on different processors with only minimal amount of communications. Targeted inverse model applications require to simulate up to 320 x 36 tracers simultaneously in adjoint mode (and much more in forward mode) for 20 years. This can be completed within about 48 hours on 640 processors (80 nodes), when running a model at 2.5 degree resolution and transporting 36 tracers per processor. Typical computation speed is about 40 sec/tracer/month at 1.1Gflops/processor.

The model demonstrated to run in parallel on up to 10 nodes and 80 processors. No performance degradation with increase of the number of nodes is observed, because all tasks including preprocessing are done in previous version on each processor. While running 22 tracers per processor the model runs independently on each node at 81% of theoretical peak performance (compared with imaginary case of "infinite" number of tracers run on single node when preprocessing overhead per tracer is minimal). Further optimization is planned to be achieved by running in parallel preprocessing and transport.

As a first application of the model, we completed simulation of the regional surface CO_2 flux pulse propagation and source-receptor relationship matrixes for the 15 years analysis of recent global carbon cycle. Several model modifications and off-line wind dataset preparation had to be done. Forward transport of monthly regional pulsed emissions was completed, which is roughly equivalent to the most detailed analysis possible at present. Increasing the detail of the analysis will be achieved by increasing number of nodes or number of runs. Results obtained with more detailed analysis are important for the whole field of the inverse modeling science, because those allow direct estimation of the errors and "aggregation" biases of the lower resolution approaches.

全球・地域スケール化学輸送モデルによる大気組成変動とその気候影響の研究

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（1）FRSGC/UCI 全球化学輸送モデル（CTM）の地球シミュレーターへの移植が成功し、全球対流圏化学モデルとしては世界で最高水準の水平解像度T63（1.9度メッシュ）、垂直解像度40層での計算が可能となった。本CTMはこれまでNEC SX5上でシングルプロセッサーで計算されていたが、本年度地球シミュレーター用に最適化されベクトル化された。地球シミュレーターに移植されたモデルによる計算結果が、従来の計算結果と一致することを検証した。

（2）化学的に不活性な長寿命温室効果ガス等の多数のトレーサーに対する逆モデル研究のため、全球大気輸送モデルの地球シミュレーターへの適応化を行った。モデルは10ノード、80プロセッサーまでの並列計算がなされ、ノード数の増加による計算結果の劣化が見られないことを検証した。このモデルの最初の応用としてCO_2の地域フラックスのシミュレーションおよび15年間のソース・リセプター関係マトリックスの解析を行った。

キーワード：化学輸送モデル、大気輸送モデル、化学的変質、逆モデリング