QUASI-NEWTON METHODS FOR ATMOSPHERIC CHEMISTRY SIMULATIONS

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Christina Mitsakou, Paul Griffiths)

Ref: Esenturk et. al., Geosci. Mod. Dev., 2018
UK Met Office United Model (UM) and UK Chemistry & Aerosol (UKCA)

• UM: ONE MODEL FOR ALL (DECADAL OZONE PREDICTIONS, CLIMATE PREDICTIONS, WEATHER FORECASTS ETC.

• UKCA SEQUENTIALLY COUPLED TO UM TRANSPORT DYNAMICS

• UKCA CONSISTS OF CHEMISTRY-AEROSOL PROCESSES, PHOTOLYSIS, EMISSIONS, WET/DRY DEPOSITIONS, CLOUDS ETC
The Problem

1 Atmospheric chemistry calculations are expensive!

In the basic test-setting (stratosphere-troposphere-no aerosol):

* A model year takes 1 day on the national supercomputer (Archer)

* Typically, UKCA takes 20-40% of computational resources*

2 Solving atmospheric chemical networks poses a “stiff problem”

Basic test-setting consists of 75 species and 283 reactions

* Orders of magnitudes of differences in the lifetime of species

* Methane > 5 years, OH
Chemical Reactions as Differential Equations (DEs)

Let \( \mathbf{c}(t) = (c_1(t), c_2(t), ..., c_N(t)) \) denote the vector of species concentrations at a given time.

\[
\frac{d\mathbf{c}}{dt} = \mathbf{f}(\mathbf{c}) = P(\mathbf{c}) - L(\mathbf{c}) + E(\mathbf{c}) - D_{\text{wet}}(\mathbf{c}) - D_{\text{dry}}(\mathbf{c}) 
\]

\[
\mathbf{c}(0) = \mathbf{a},
\]

\( P(\mathbf{c}) \): Production terms
\( L(\mathbf{c}) \): Loss terms
\( E(\mathbf{c}) \): Emission terms
\( D_{\text{wet}}(\mathbf{c}) \): Wet deposition terms
\( D_{\text{dry}}(\mathbf{c}) \): Dry deposition terms
Numerical Methods for Solving DEs

1 EXPLICIT METHODS
- DIRECT, QUICK AND HANDY
- LESS STABLE

Example: FORWARD EULER
\[ c(t + \Delta t) = c(t) + f(c(t))\Delta t \]

2 IMPLICIT METHODS
- INDIRECT AND LABORIOUS
- MORE STABLE

Example: BACKWARD EULER
\[ c(t + \Delta t) = c(t) + f(c(t + \Delta t))\Delta t \]

where \( \Delta t \) is the time-step of the numerical scheme
Time Integration in the UKCA: The ASAD Framework

THE UKCA VERSION OF THE ASAD PACKAGE

- USES BACKWARD EULER WITH FIXED TIME-STEP
- USES NEWTON-RAPHSON ALGORITHM TO SOLVE

THE NONLINEAR ALGEBRAIC EQUATION:

\[ F(c(t)) = \frac{c(t) - c_0}{\Delta t} - f(c(t)) = 0. \]
Newton-Raphson Algorithm

Newton-Raphson Algorithm computes the solution ITERATIVELY taking higher dimensional derivatives (The Jacobian) at each step and solving the linear equation

\[
J(c^k)(\Delta c^k) = -F(c^k)
\]

\[
\Delta c^k = c^{k+1} - c^k
\]

VERY COSTLY!
Newton-Raphson (NR) X Quasi-Newton (QN)


INSTEAD OF NR, USE QUASI-NEWTON (QN) STEPS!
(APPROXIMATE DERIVATIVES FOR THE JACOBIAN)
QN IMPLEMENTATION FOR THE UKCA

TWO-FOLD SAVINGS WITH QN STEPS

1) AVOID RECONSTRUCTION OF THE JACOBIAN

2) RECYCLE THE INFORMATION WITHIN AN ITERATION TO FAST SOLVE THE LINEAR EQUATION
UKCA Box-Model (UKCA_BOX)

UKCA_BOX: Highly controlled simplified environment for simulation of chemical reactions

Developed by Scott A. Nicholls

ADVANTAGES
1) ALLOWS ONE TO OPTIMISE THE MODEL OPTIONS BEFORE RUNNING A FULL UM SIMULATION
2) RUNS ON A SINGLE PROCESSOR CORE: MUCH CHEAPER & FASTER THAN FULL SIMULATION!
An Urban Scenario with UKCA_BOX

WHY URBAN SCENARIO?:
Better representative atmospheric environment

<table>
<thead>
<tr>
<th>Method</th>
<th>CPU time for 1000 calls</th>
<th>Wallclock time 1000 calls</th>
</tr>
</thead>
<tbody>
<tr>
<td>Full Newton Raphson</td>
<td>160 ± 3.1 ms</td>
<td>157 ± 1.8 ms</td>
</tr>
<tr>
<td>Quasi-Newton Method</td>
<td>42 ± 0.71 ms</td>
<td>42.9 ± 0.15 ms</td>
</tr>
</tbody>
</table>

Ref: Esenturk et. al., Geo. Mod. Dev., 2018
# Full UM-UKCA Simulations

QN METHOD OFFERS TWO-FOLD ADVANTAGE

## Advantage 1: Increased speed by up to %13 in chemistry routines

<table>
<thead>
<tr>
<th>Scheme</th>
<th>Pure Chemistry</th>
<th>Chemistry &amp; Aerosol</th>
<th>Pure Chemistry</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cores</td>
<td>432</td>
<td>432</td>
<td>216</td>
</tr>
<tr>
<td>Simulation</td>
<td>CNTL</td>
<td>QN2-3</td>
<td>CNTL</td>
</tr>
<tr>
<td>Dynamics</td>
<td>12123 ± 22</td>
<td>12099 ± 23</td>
<td>15297 ± 27</td>
</tr>
<tr>
<td>Chemistry</td>
<td>4228 ± 26</td>
<td>3678 ± 16</td>
<td>4123 ± 19</td>
</tr>
<tr>
<td>Chemistry Speed-up (%)</td>
<td>13.00</td>
<td>12.74</td>
<td>13.48</td>
</tr>
<tr>
<td>UM Speed-up (%)</td>
<td>2.33</td>
<td>1.81</td>
<td>3.59</td>
</tr>
</tbody>
</table>

## Advantage 2: Increased robustness in tough atmospheric environments (e.g. boundary layers)

<table>
<thead>
<tr>
<th>Scheme</th>
<th>Number of Cores</th>
<th>Simulation</th>
<th>Number of halving steps</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pure Chemistry</td>
<td>216</td>
<td>CNTL</td>
<td>457344</td>
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<tr>
<td></td>
<td>432</td>
<td>QN2-3</td>
<td>270101</td>
</tr>
<tr>
<td>Chemistry &amp; Aerosol</td>
<td>432</td>
<td>CNTL</td>
<td>436048</td>
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<tr>
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<td></td>
<td>QN2-3</td>
<td>256019</td>
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Full UM-UKCA Simulations

QN METHOD DOES NOT AFFECT ACCURACY

Define Normalised Mean Absolute Difference (NMAD) and Normalised Root Mean Square Difference (NRMSD)

\[ NMAD_S = \frac{\sum_i |c_{S,nr}^i(T) - c_{S,qn}^i(T)|}{\sum_i |c_{S,nr}^i(T)|} \]

\[ NRMSD_S = \sqrt{\frac{\sum_i |c_{S,nr}^i(T) - c_{S,qn}^i(T)|^2}{\sum_i |c_{S,nr}^i(T)|^2}} \]

<table>
<thead>
<tr>
<th>Chemistry</th>
<th>Species</th>
<th>Comparison</th>
<th>NMAD</th>
<th>NMRSD</th>
<th>NMB</th>
</tr>
</thead>
<tbody>
<tr>
<td>No Aerosol (432 cores)</td>
<td>OH</td>
<td>CNTL vs QN2-3</td>
<td>3.6986 10^{-8}</td>
<td>3.6019 10^{-8}</td>
<td>3.0382 10^{-9}</td>
</tr>
<tr>
<td>No Aerosol (432 cores)</td>
<td>Ozone</td>
<td>CNTL vs QN2-3</td>
<td>8.8374 10^{-7}</td>
<td>8.9908 10^{-7}</td>
<td>7.3761 10^{-7}</td>
</tr>
</tbody>
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Comparison of Newton-Raphson Vs Quasi-Newton method by the metrics NMAD and NMRSD (for 20-year model run)
THANK YOU