QUASI-NEWTON METHODS FOR ATMOSPHERIC CHEMISTRY SIMULATIONS

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UK Met Office United Model (UM) and UK Chemistry & Aerosol (UKCA)

- **UM**: ONE MODEL FOR ALL (DECADAL OZONE PREDICTIONS, CLIMATE PREDICTIONS, WEATHER FORECASTS ETC.
- UM CONSISTS OF TRANSPORT DYNAMICS, CONVECTION, PHOTOLYSIS, CHEMISTRY-AEROSOL PROCESSES (UKCA) ETC
- **UKCA** CONSISTS OF CHEMISTRY-AEROSOL PROCESSES, EMISSIONS, WET/DRY DEPOSITIONS ETC
- **UKCA IS SEQUENTIALLY COUPLED TO UM TRANSPORT DYNAMICS**

Two Problems: Speed and Robustness

1 ATMOSPHERIC CHEMISTRY & AEROSOL 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)

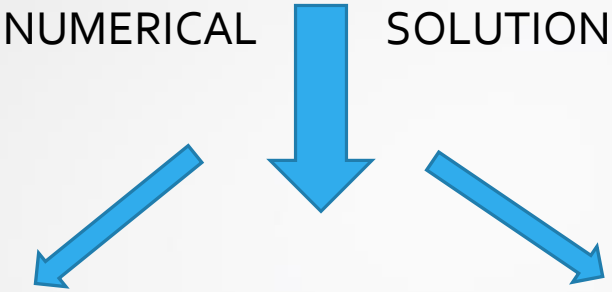
Let $\boldsymbol{c}(t) = (c_1(t), c_2(t), \ldots, c_N(t))$ denote the vector of species concentrations at a given time

$$\frac{d\boldsymbol{c}}{dt} = \boldsymbol{f}(\boldsymbol{c}) = \boldsymbol{P}(\boldsymbol{c}) - \boldsymbol{L}(\boldsymbol{c}) + \boldsymbol{E}(\boldsymbol{c}) - \boldsymbol{D_{wet}}(\boldsymbol{c}) - \boldsymbol{D_{dry}}(\boldsymbol{c}) \qquad (1)$$

$$\boldsymbol{c}(0) = \boldsymbol{a}, \qquad (2)$$

$\boldsymbol{P}(\boldsymbol{c})$: Production terms
$\boldsymbol{L}(\boldsymbol{c})$: Loss terms
$\boldsymbol{E}(\boldsymbol{c})$: Emission terms
$\boldsymbol{D_{wet}}(\boldsymbol{c})$: Wet deposition terms
$\boldsymbol{D_{dry}}(\boldsymbol{c})$: Dry deposition terms

Numerical Methods for Solving DEs



1 EXPLICIT METHODS

- DIRECT, QUICK AND HANDY
- LESS STABLE

Example: FORWARD EULER

$$\boldsymbol{c}(t+\Delta t) = \boldsymbol{c}(t) + f(\boldsymbol{c}(t))\Delta t$$

2 IMPLICIT METHODS

- INDIRECT AND LABORIOUS
- MORE STABLE

Example: BACKWARD EULER

$$\boldsymbol{c}(t+\Delta t) = \boldsymbol{c}(t) + f(\boldsymbol{c}(t+\Delta t))\Delta t$$

where Δt 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:

$$\boldsymbol{F}(\boldsymbol{c}) = \frac{\boldsymbol{c} - \boldsymbol{c}_*}{\Delta t} - \boldsymbol{f}(\boldsymbol{c}) = 0.$$

Newton-Raphson Algorithm

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

1st STEP $\mathbf{J}(\boldsymbol{c}^k)(\boldsymbol{c}^k) = \mathbf{DF}(\boldsymbol{c}^k) \equiv Derivative\ of\ F$

2nd STEP $\mathbf{J}(\boldsymbol{c}^k)(\Delta\boldsymbol{c}^k) = -\mathbf{F}(\boldsymbol{c}^k)$ ⟶ *Solve linear system*

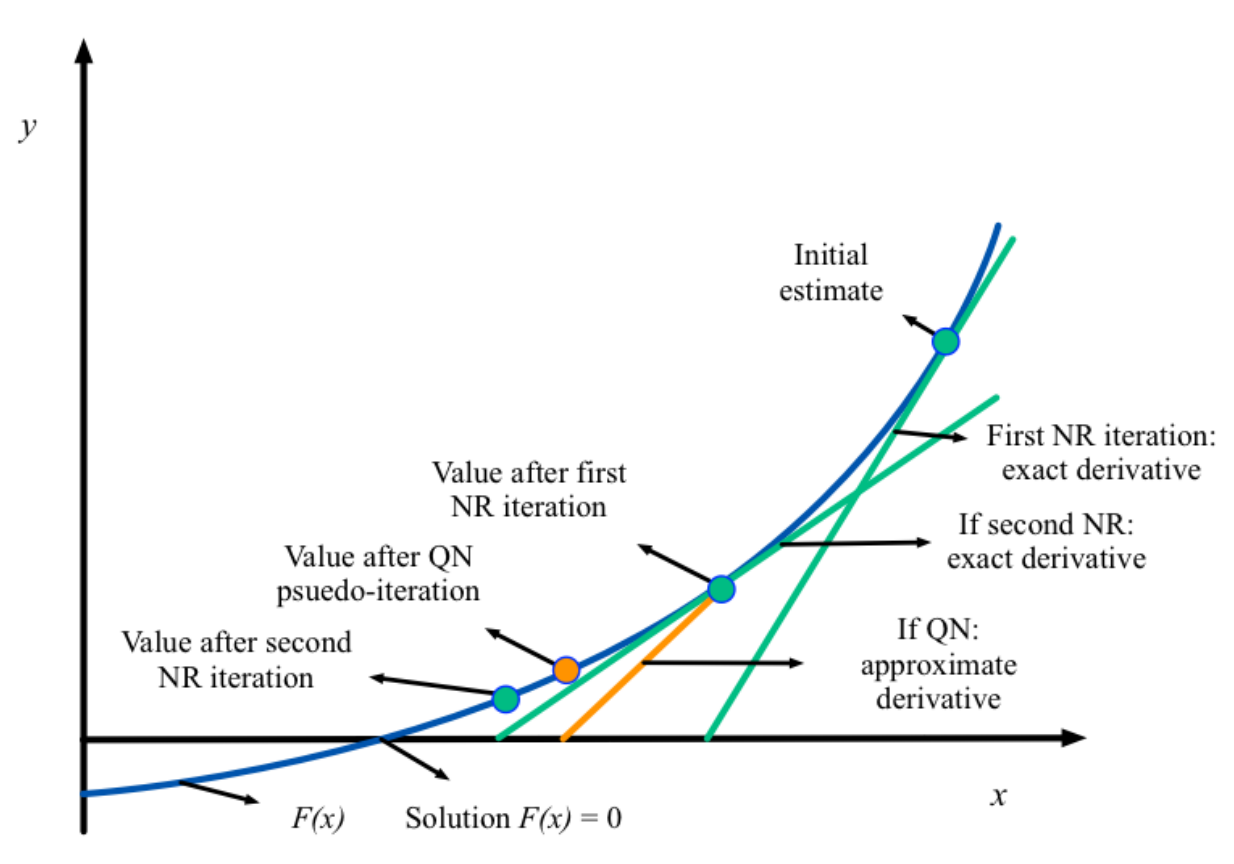
$$\Delta\boldsymbol{c}^k = \boldsymbol{c}^{k+1} - \boldsymbol{c}^k$$

VERY COSTLY !

Newton-Raphson (NR) X Quasi-Newton (QN)

There are additional steps in the QN algorithm BUT the numerical steps are **SIMPLER AND EFFICIENT**

Broyden (1965),
Shanno (1970),
Fletcher (1970),
Goldfarb (1971),
Davidon (1991).



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

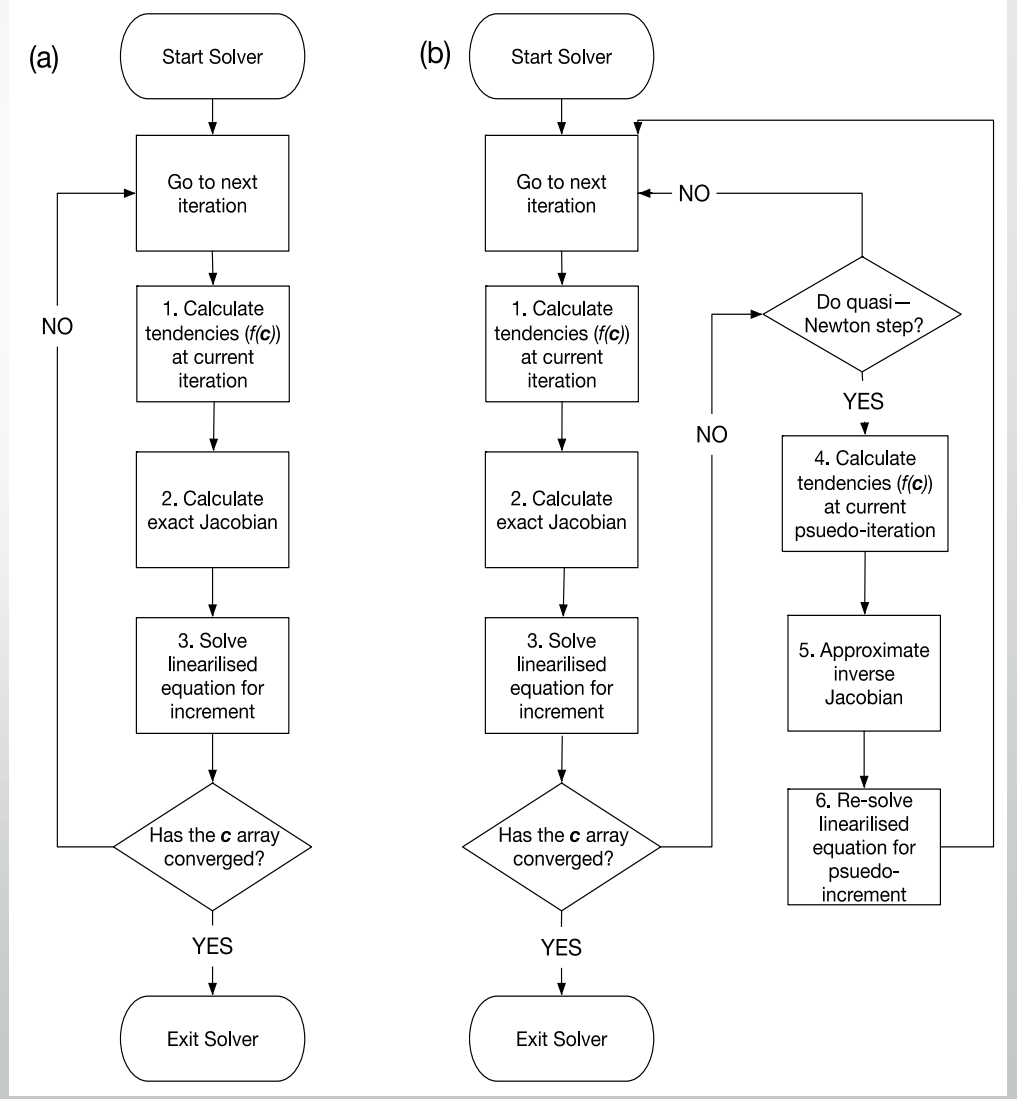
Flow Chart for the QN Implementation

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 (U. Cambridge, 2017)

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 !**

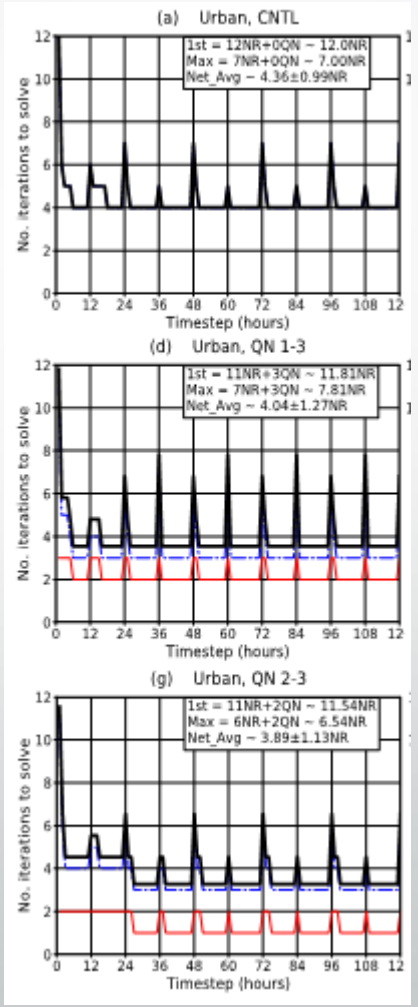
An Urban Scenario with UKCA_BOX

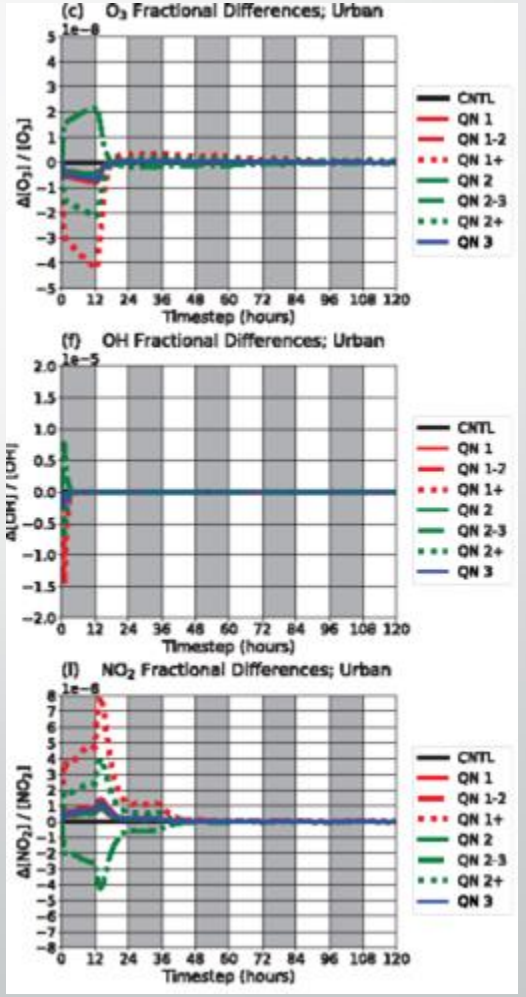
WHY URBAN SCENARIO?:

Better representative of atmospheric environments

	Full Newton Raphson Method	Quasi-Newton Method
CPU time for 1000 calls	160 ± 3.1 ms	42 ± 0.71 ms
Wallclock time 1000 calls	157 ± 1.8 ms	42.9 ± 0.15 ms

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

Scheme	Pure Chemistry		Chemistry & Aerosol		Pure Chemistry	
Cores	432		432		216	
Simulation	CNTL	QN2-3	CNTL	QN2-3	CNTL	QN2-3
Dynamics	12123 ± 22	12099 ± 23	15117 ± 28	15297 ± 27	18881 ± 27	18743 ± 30
Chemistry	4228 ± 26	3678 ± 16	4725 ± 28	4123 ± 19	9102 ± 96	7875 ± 75
Chemistry Speed-up (%)	13.00		12.74		13.48	
UM Speed-up (%)	2.33		1.81		3.59	

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

Scheme	Number of Cores	Simulation	Number of halving steps
Pure Chemistry	216	CNTL	457344
		QN2-3	270101
	432	CNTL	436048
		QN2-3	256019
Chemistry & Aerosol	432	CNTL	544532
		QN2-3	328836

Ref: Esenturk et. al., Geo. Mod. Dev., 2018

Full UM-UKCA Simulations

QN METHOD DOES NOT AFFECT ACCURACY

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

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

$$\mathrm{NRMSD}_S = \sqrt{\frac{\sum_i |c_{S,nr}{}^i(T) - c_{S,qn}{}^i(T)|^2}{\sum_i |c_{S,nr}{}^i(T))|^2}}$$

Chemistry	Species	Comparison	NMAD	NMRSD	NMB
No Aerosol (432 cores)	OH	CNTL vs QN2-3	$3.6986\ 10^{-8}$	$3.6019\ 10^{-8}$	$3.0382\ 10^{-9}$
No Aerosol (432 cores)	Ozone	CNTL vs QN2-3	$8.8374\ 10^{-7}$	$8.9908\ 10^{-7}$	$7.3761\ 10^{-7}$

Comparison of Newton-Raphson Vs Quasi-Newton method by the metrics NMAD and NMRSD (for 20-year model run)

THANK YOU