Analysis Methods in Atmospheric and Oceanic Science

AOSC 652

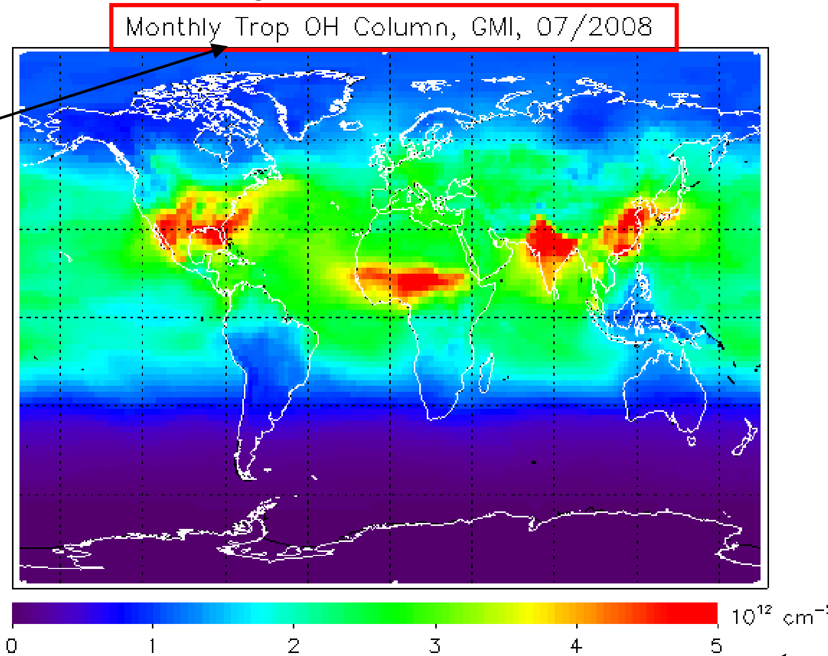
Numerical Integration

Week 6, Day 1

3 Oct 2016

AOSC 652: Analysis Methods in AOSC

Trop: Troposphere



OH Column: Units of 10^{12} molecules cm^{-2} OR 10^{12} cm^{-2}

How is Trop OH column from a model such as the Goddard "Global Modeling Initiative" (GMI) Chemical Transport Model (CTM) found ???

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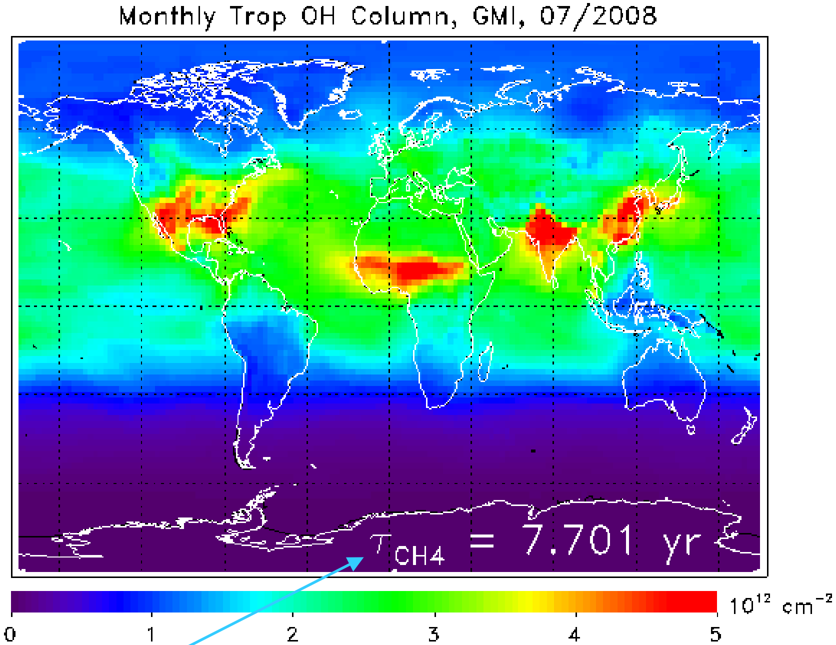
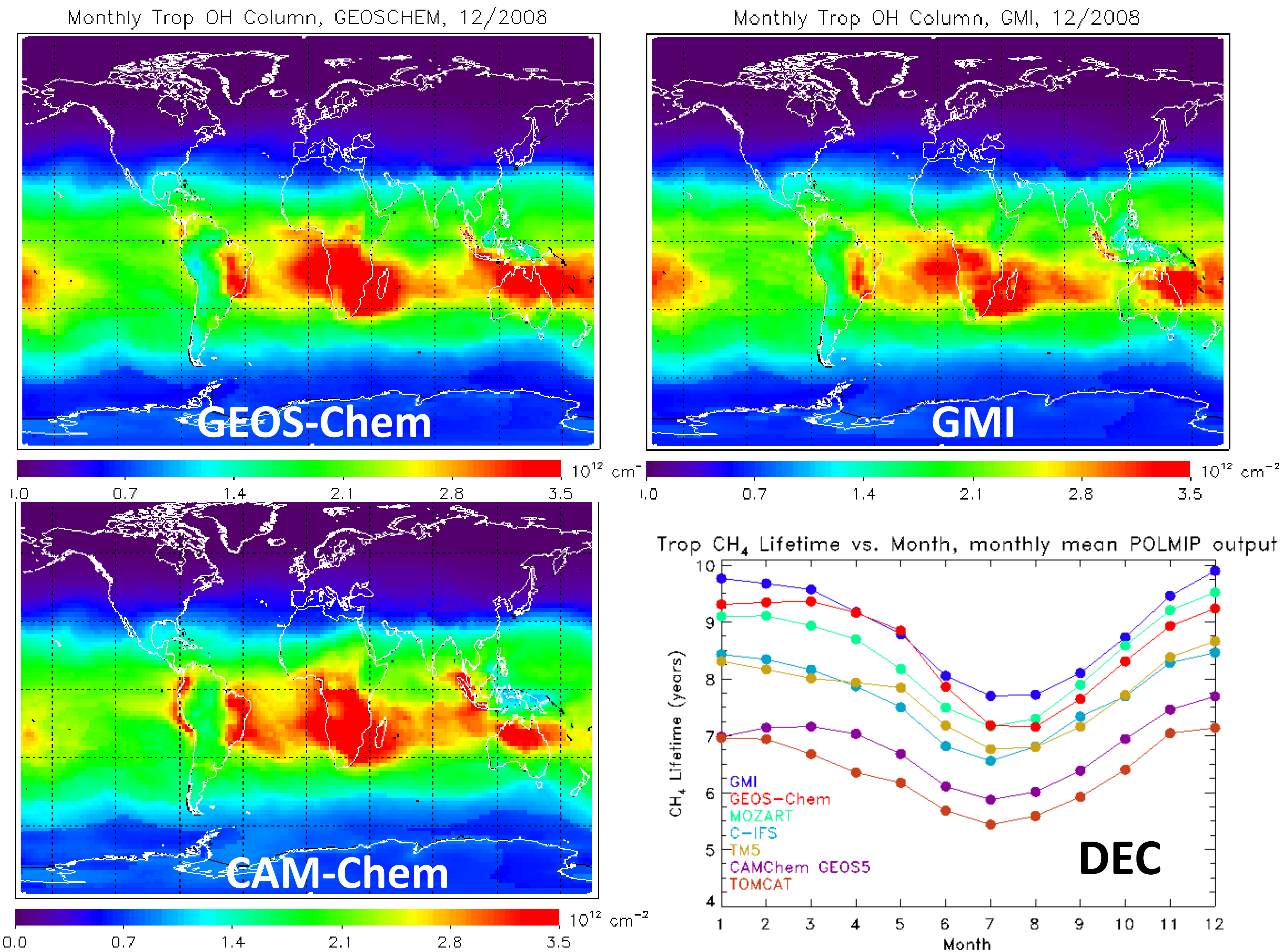


τ_{CH4} : CH_4 Lifetime with respect to loss by reaction w/ tropospheric OH

How found ?!?



Monthly Trop OH Column, GEOSCHEM, 12/2008
GEOS-Chem
0.7
1.4
2.1
2.8
3.5
10^{12} cm
Monthly Trop OH Column, GMI, 12/2008
GMI
0.7
1.4
2.1
2.8
3.5
10^{12} cm^{-2}
CAM-Chem
0.0
0.7
1.4
2.1
2.8
3.5
10^{12} cm^{-2}
Trop CH_4 Lifetime vs. Month, monthly mean POLMIP output
CH_4 Lifetime (years)
Month
GMI
GEOS−Chem
MOZART
C−IFS
TM5
CAMChem GEOS5
TOMCAT
DEC

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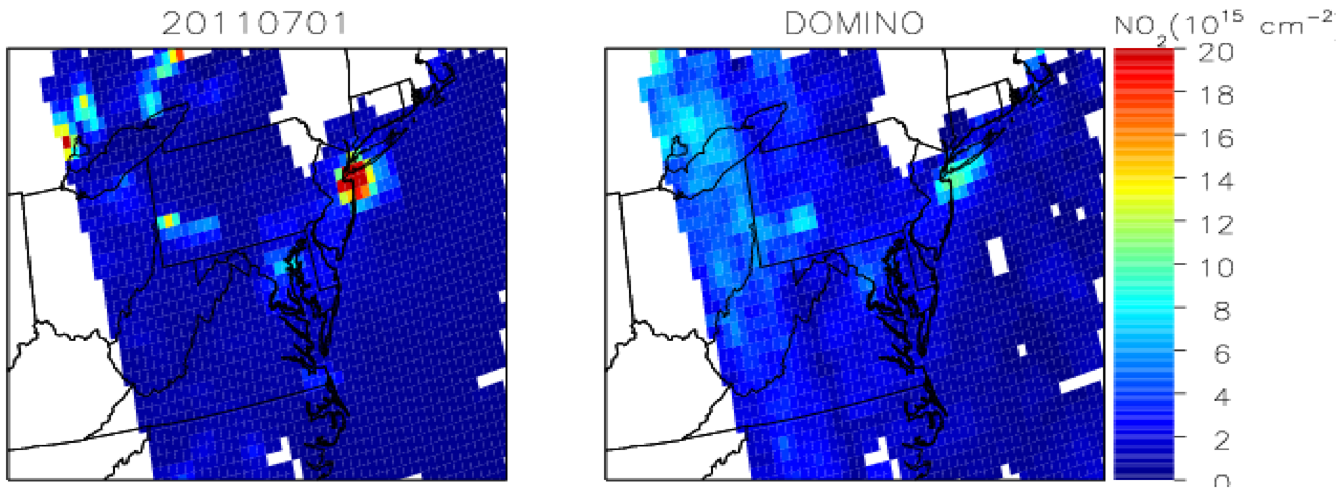
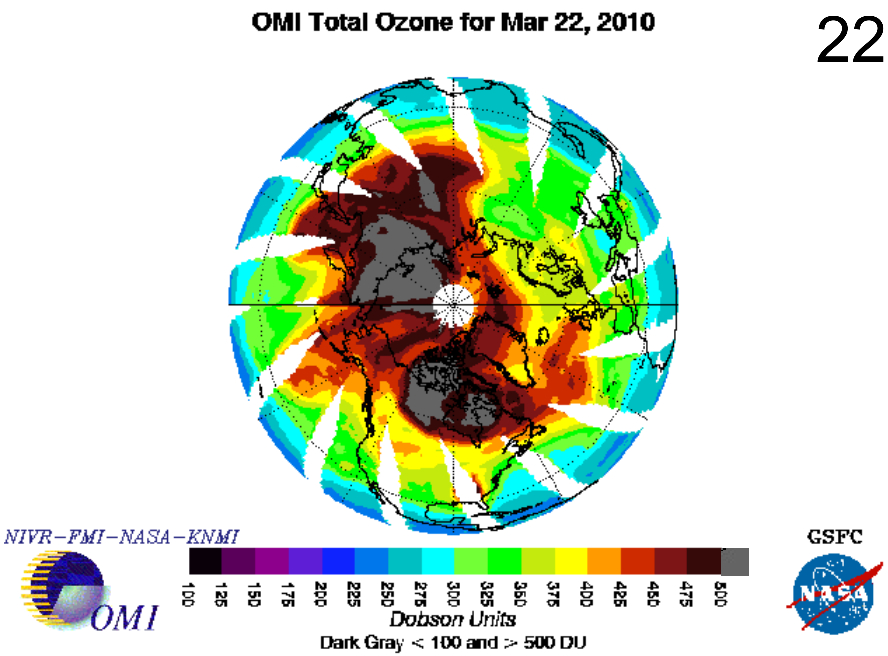
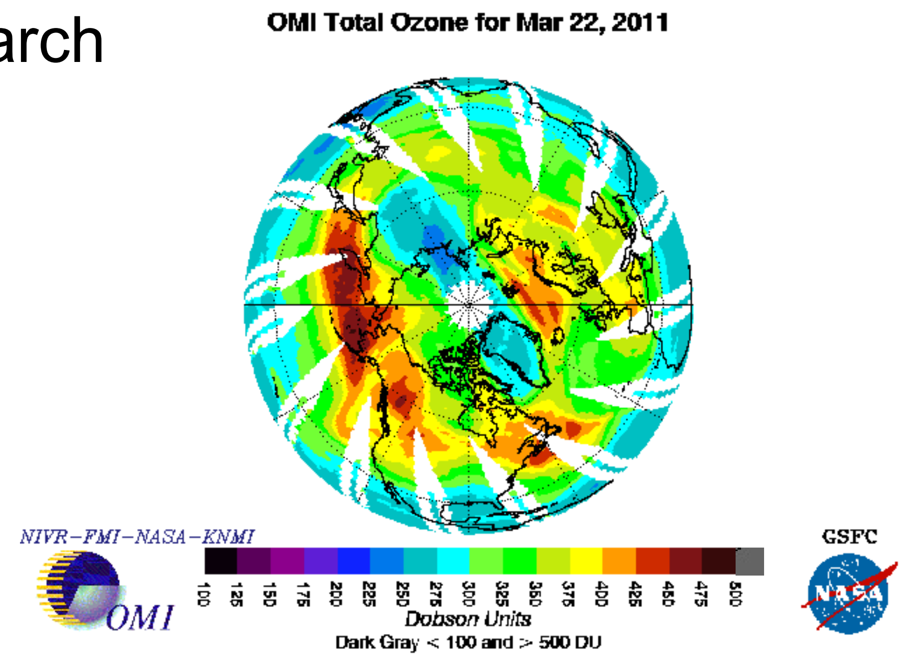
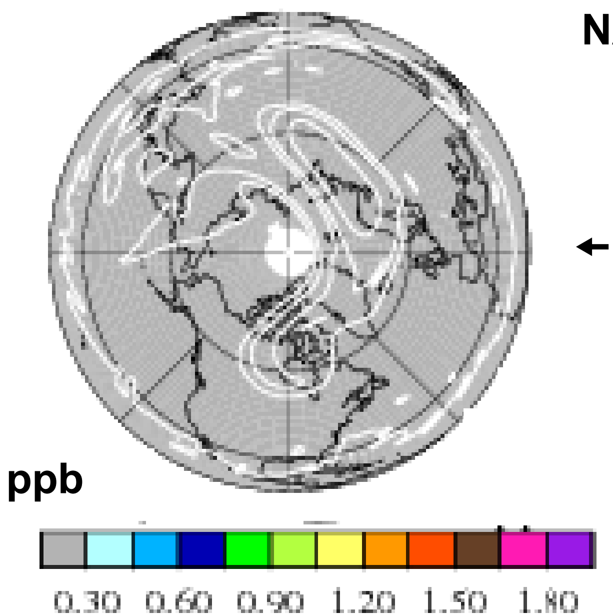
Air Quality Model | **Satellite Data**



22 March

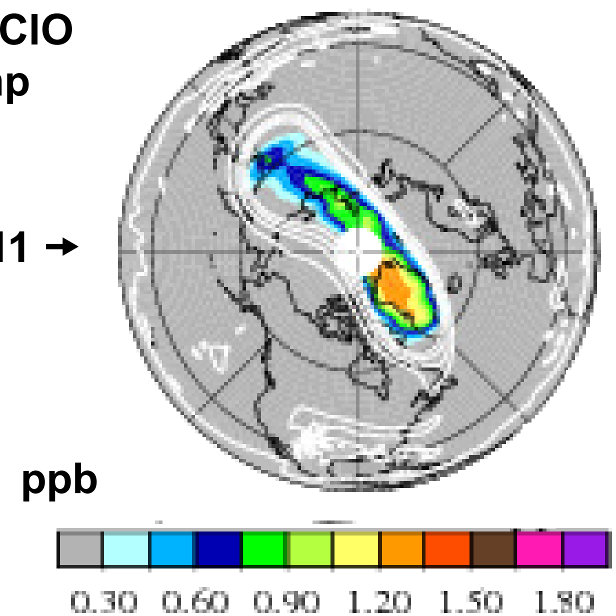






NASA Aura MLS ClO
490 K pot'l temp
~18 km

22 March
← 2010 2011 →



Unprecedented Arctic ozone loss in 2011

Gloria L. Manney[1,2], Michelle L. Santee[1], Markus Rex[3], Nathaniel J. Livesey[1], Michael C. Pitts[4], Pepijn Veefkind[5,6], Eric R. Nash[7], Ingo Wohltmann[3], Ralph Lehmann[3], Lucien Froidevaux[1], Lamont R. Poole[8], Mark R. Schoeberl[9], David P. Haffner[7], Jonathan Davies[10], Valery Dorokhov[11], Hartwig Gernandt[3], Bryan Johnson[12], Rigel Kivi[13], Esko Kyrö[13], Niels Larsen[14], Pieternel F. Levelt[5,6,15], Alexander Makshtas[16], C. Thomas McElroy[10], Hideaki Nakajima[17], Maria Concepción Parrondo[18], David W. Tarasick[10], Peter von der Gathen[3], Kaley A. Walker[19] & Nikita S. Zinoviev[16]

Since the emergence of the Antarctic 'ozone hole' in the 1980s[1] and elucidation of the chemical mechanisms[2–5] and meteorological conditions[6] involved in its formation, the likelihood of extreme ozone depletion over the Arctic has been debated. Similar processes are at work in the polar lower stratosphere in both hemispheres, but differences in the evolution of the winter polar vortex and associated polar temperatures have in the past led to vastly disparate degrees of springtime ozone destruction in the Arctic and Antarctic. We show that chemical ozone loss in spring 2011 far exceeded any previously observed over the Arctic. For the first time, sufficient loss occurred to reasonably be described as an Arctic ozone hole.

doi:10.1038/nature10556
2 October 2011

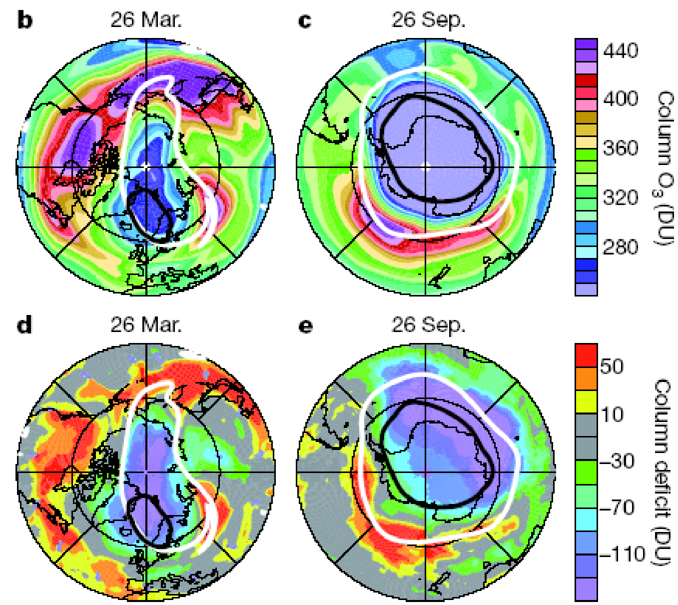


Figure 5 | Total column ozone. **a**, Time series of the fraction of 460 K vortex area with total ozone below 275 Dobson units (DU) in February–April in the Arctic (bottom axis), and in August–October in the Antarctic (top axis). Line colours/shading as in Fig. 1. 2005–2011 values are from OMI; earlier values are from TOMS (Total Ozone Mapping Spectrometer) instruments[50]. Maps show OMI total ozone (**b**, **c**) and ozone deficit (**d**, **e**) in the Arctic (Antarctic) on 26 March 2011 (26 September 2010). Overlays as in Fig. 2 but at 460 K.

Unprecedented Arctic ozone loss in 2011

Gloria L. Manney[1,2], Michelle L. Santee[1], Markus Rex[3], Nathaniel J. Livesey[1], Michael C. Pitts[4], Pepijn Veefkind[5,6], Eric R. Nash[7], Ingo Wohltmann[3], Ralph Lehmann[3], Lucien Froidevaux[1], Lamont R. Poole[8], Mark R. Schoeberl[9], David P. Haffner[7], Jonathan Davies[10], Valery Dorokhov[11], Hartwig Gernandt[3], Bryan Johnson[12], Rigel Kivi[13], Esko Kyrö[13], Niels Larsen[14], Pieternel F. Levelt[5,6,15], Alexander Makshtas[16], C. Thomas McElroy[10], Hideaki Nakajima[17], Maria Concepción Parrondo[18], David W. Tarasick[10], Peter von der Gathen[3], Kaley A. Walker[19] & Nikita S. Zinoviev[16]

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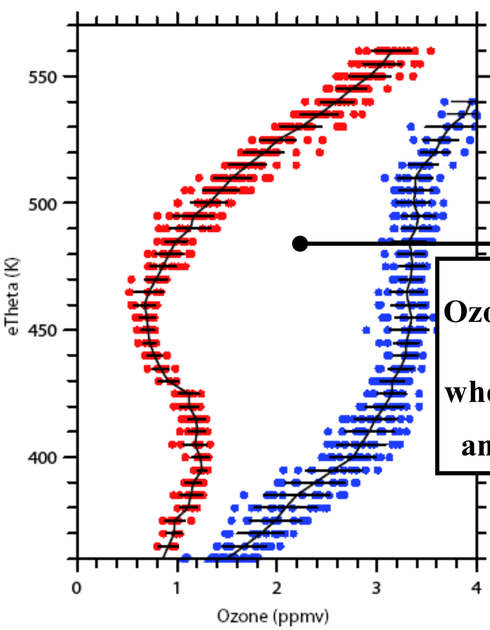
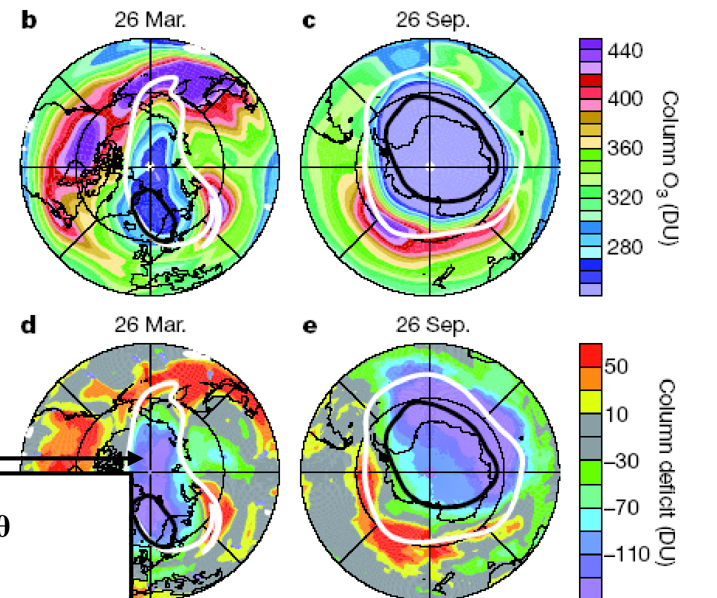




$$\text{Ozone Deficit} = \text{Factor} \times \int_{\theta_{LOW}}^{\theta_{HIGH}} \left\{ O_3^{*}(\theta) - O_3(\theta) \right\} d\theta$$

where O_3 (θ) is measured profile (RED)

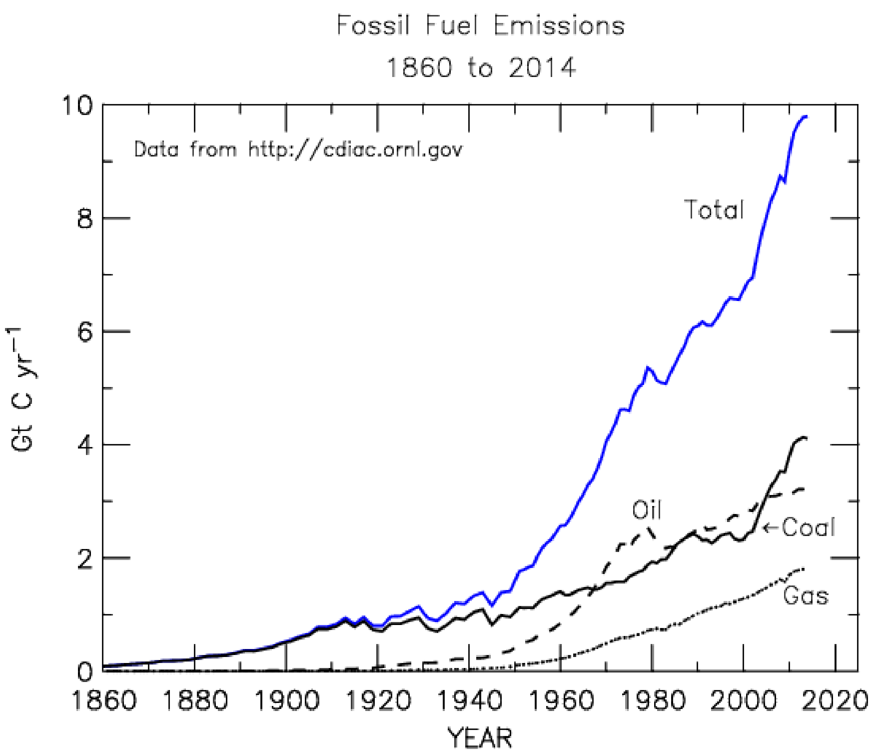
and O_3^{*}(θ) is profile without any chemical loss (BLUE)

...lumn ozone. **a**, Time series of the fraction of 460 K vortex ...he below 275 Dobson units (DU) in February–April in the Arctic (bottom axis), and in August–October in the Antarctic (top axis). Line colours/shading as in Fig. 1. 2005–2011 values are from OMI; earlier values are from TOMS (Total Ozone Mapping Spectrometer) instruments[50]. Maps show OMI total ozone (**b**, **c**) and ozone deficit (**d**, **e**) in the Arctic (Antarctic) on 26 March 2011 (26 September 2010). Overlays as in Fig. 2 but at 460 K.

Numerical Integration

Why else might you need to compute an integral ?

Calculate carbon emissions to compare with change in atmospheric CO_2



CO_2 emission, 1959 to 2014 = 323.6 Gt C

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Numerical Integration

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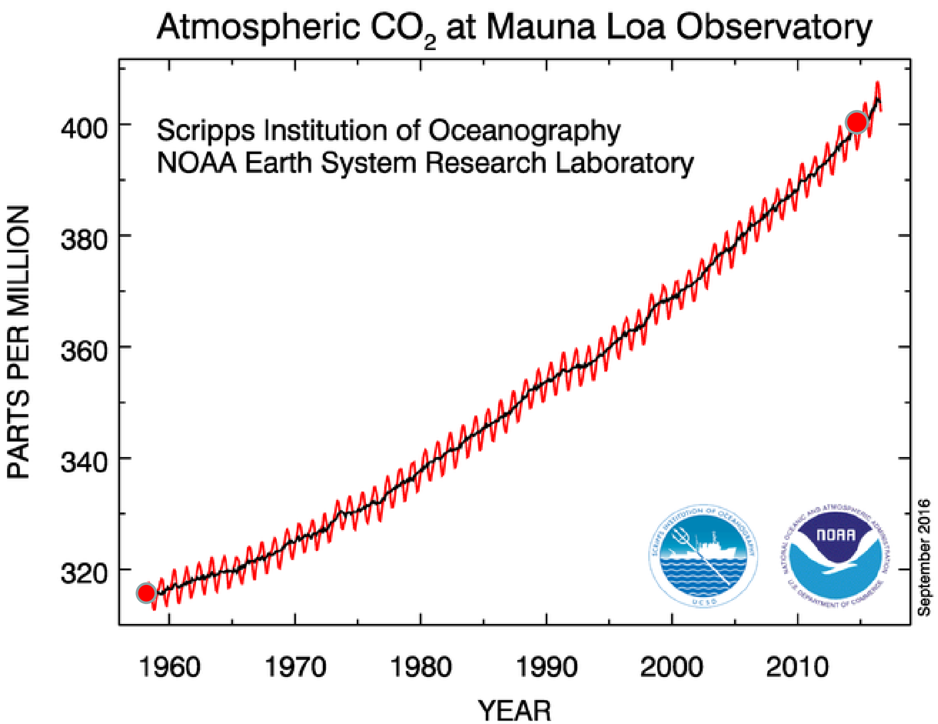

CO_2 emission, 1959 to 2014 = 323.6 Gt C

Change in atmospheric CO_2, 1959 to 2014 = 82.64 ppm
82.64 ppm × 2.18 Gt C / ppm CO_2 = 180.16 Gt C

About half of the CO_2 released by combustion of fossil fuels stays in the atmosphere:

Legacy of Charles Keeling, Scripps Institution of Oceanography, La Jolla, CA
http://www.esrl.noaa.gov/gmd/ccgg/trends/co2_data_mlo.html

Numerical Integration

Why might you need to compute an integral ?

Heat Balance in Ocean:

$$\int_0^t Q_{OCEAN-WARMING}\ dt =$$

$$\int_0^t \left(Q_{SOLAR} - Q_{IR\ RADIATION} - Q_{EVAPORATION} - Q_{SENSIBLE\ \ HEAT\ \ LOSS/GAIN} \right) dt$$

Numerical Integration

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$$\int_0^t \left(Q_{SOLAR} - Q_{IR\ RADIATION} - Q_{EVAPORATION} - Q_{SENSIBLE\ \ HEAT\ \ LOSS/GAIN} \right) dt$$

This heat then affects temperature in a particular ocean layer via:

$$\int_0^t Q_{OCEAN-WARMING} \; dt = \int_0^Z c_p \, \rho \, \Delta \mathrm{T} \, dz$$

Numerical Integration

Also known as “quadrature”

Why might you need to compute an integral ?

Find pressure based on the mass of the overlying atmosphere:

$$p(z) = \int_{z}^{\infty} g \ \rho \ \mathrm{d}z$$

Find dynamic height D of ocean based on specific volume α:

$$D = \int_{p_1}^{p_2} \alpha \ \mathrm{d}p$$

Numerical Integration

Trapezoidal Rule:

$$\int_{x_1}^{x_N} f(x)\, dx \;\approx\; \sum_{i=1}^{N-1} (x_{i+1} - x_i)\, \frac{f(x_{i+1}) + f(x_i)}{2}$$

Numerical Integration

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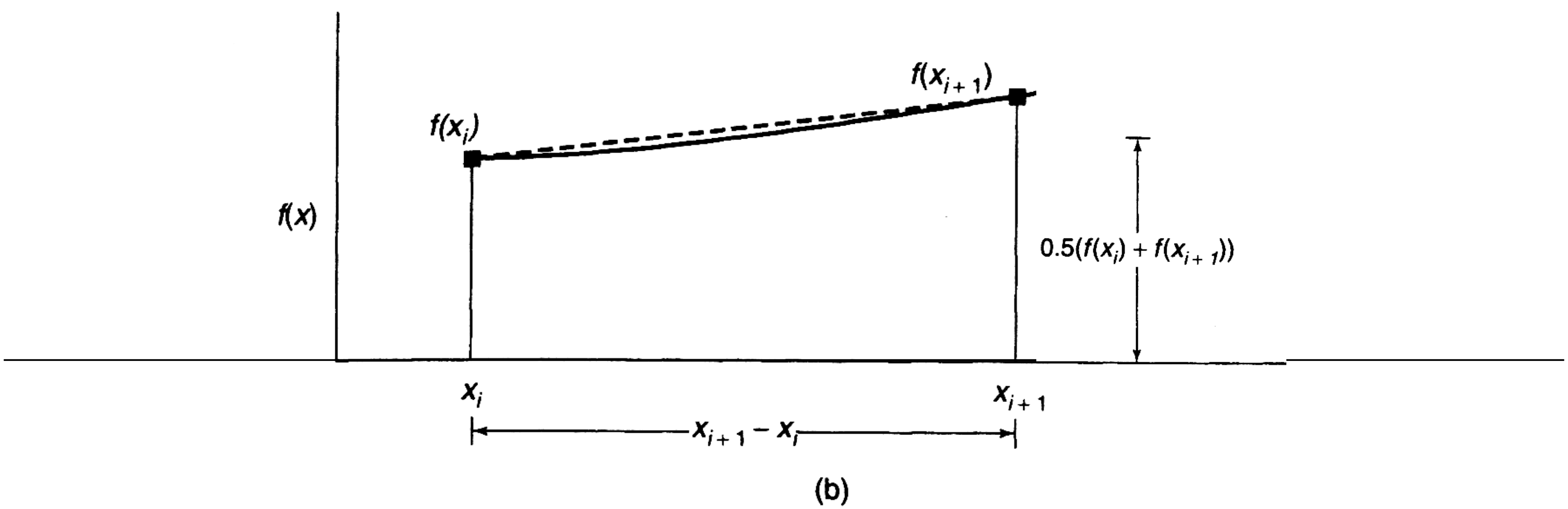


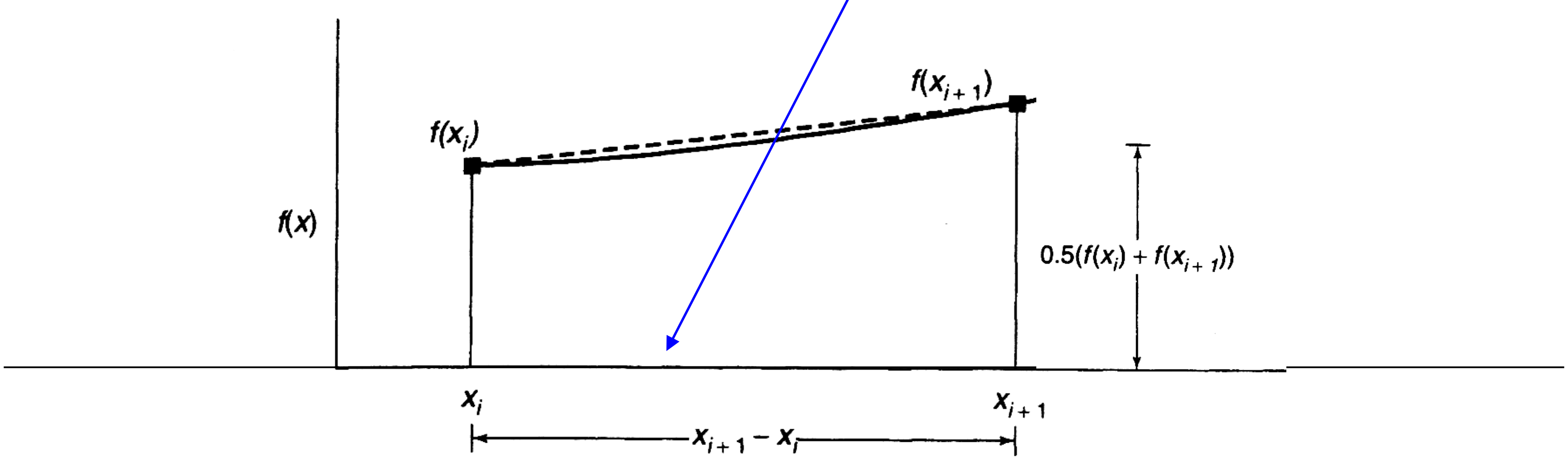
Analysis Methods for Engineers, Ayyub and McCuen

Numerical Integration

Trapezoidal Rule:

$$\int_{x_1}^{x_N} f(x)\,dx \approx \sum_{i=1}^{N-1} (x_{i+1} - x_i)\,\frac{f(x_{i+1}) + f(x_i)}{2}$$

Base of trapezoid



(b)

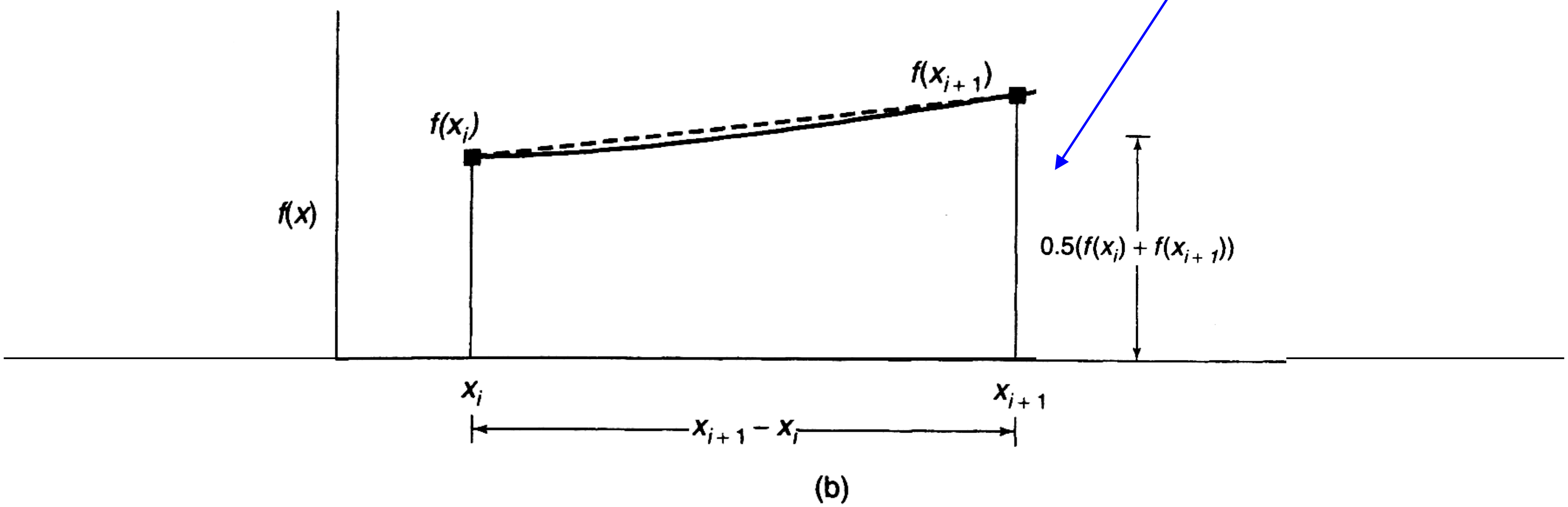
Analysis Methods for Engineers, Ayyub and McCuen

Numerical Integration

Trapezoidal Rule:

$$\int_{x_1}^{x_N} f(x)\, dx \approx \sum_{i=1}^{N-1} (x_{i+1} - x_i)\ \frac{f(x_{i+1}) + f(x_i)}{2}$$

Avg height of end points



Analysis Methods for Engineers, Ayyub and McCuen

Numerical Integration

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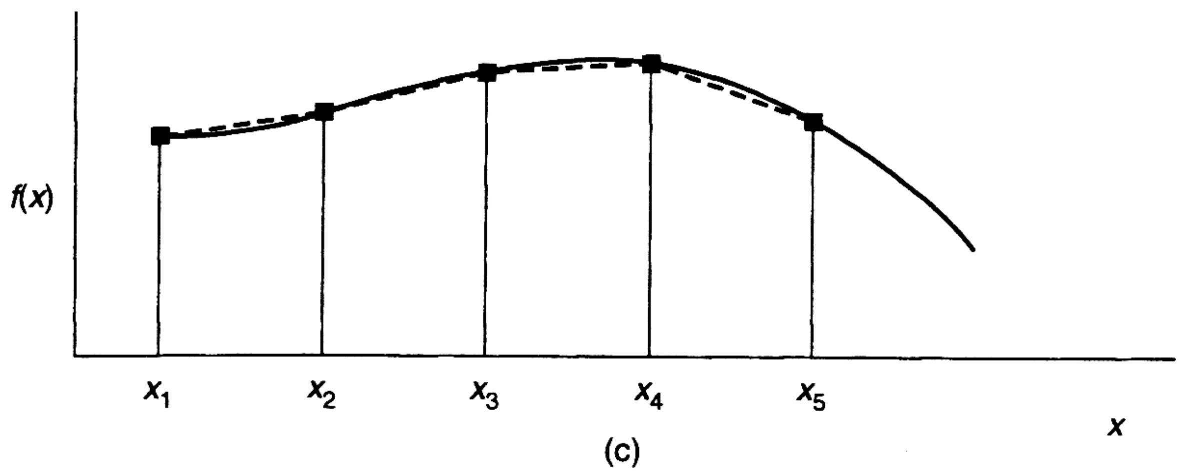
$$\int_{x_1}^{x_N} f(x)\,dx \;\approx\; \sum_{i=1}^{N-1} (x_{i+1} - x_i)\,\frac{f(x_{i+1}) + f(x_i)}{2}$$

Case where integration using the trapezoidal rule should work well:



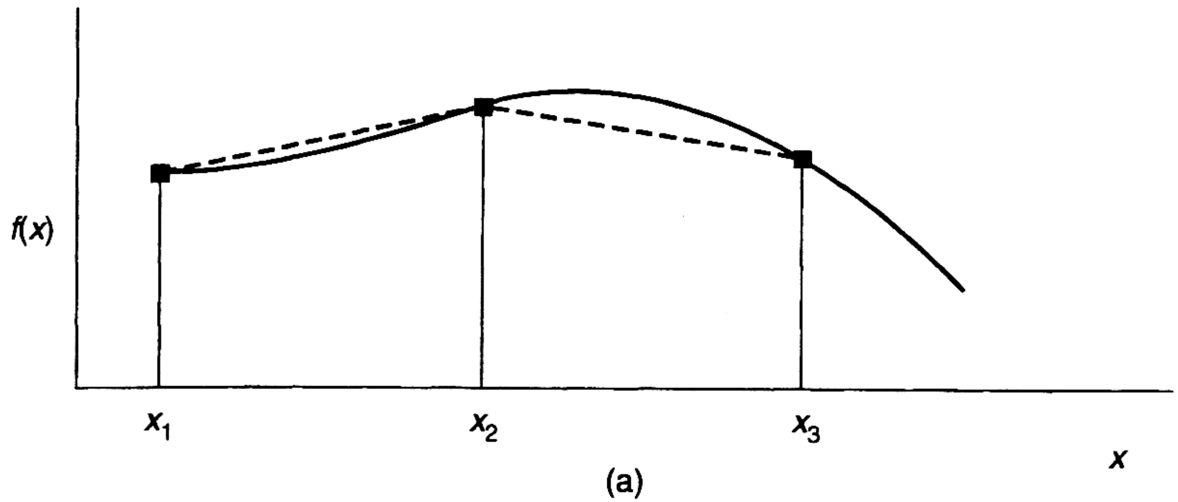
Analysis Methods for Engineers, Ayyub and McCuen

Numerical Integration

Trapezoidal Rule:

$$\int_{x_1}^{x_N} f(x)\, dx \approx \sum_{i=1}^{N-1} (x_{i+1} - x_i)\, \frac{f(x_{i+1}) + f(x_i)}{2}$$

Case where integration using the trapezoidal rule may not work well:



Analysis Methods for Engineers, Ayyub and McCuen

Numerical Integration

Trapezoidal Rule:

$$\int_{x_1}^{x_N} f(x)\,dx \approx \sum_{i=1}^{N-1} (x_{i+1} - x_i)\,\frac{f(x_{i+1}) + f(x_i)}{2}$$

Error order d^2f/dx^2: i.e., second derivative of function evaluated at some place in the interval

Hence, trapezoidal rule is exact for any function whose second derivative is identically zero.

Numerical Integration

Simpson's Rule:

$$\int_{x_1}^{x_N} f(x)\, dx \;\approx\; \sum_{i=1,\;3,\;5}^{N-2} \frac{x_{i+2} - x_i}{2} \; \frac{f(x_{i+2}) + 4f(x_{i+1}) + f(x_i)}{3}$$

What is the basis of this formula?

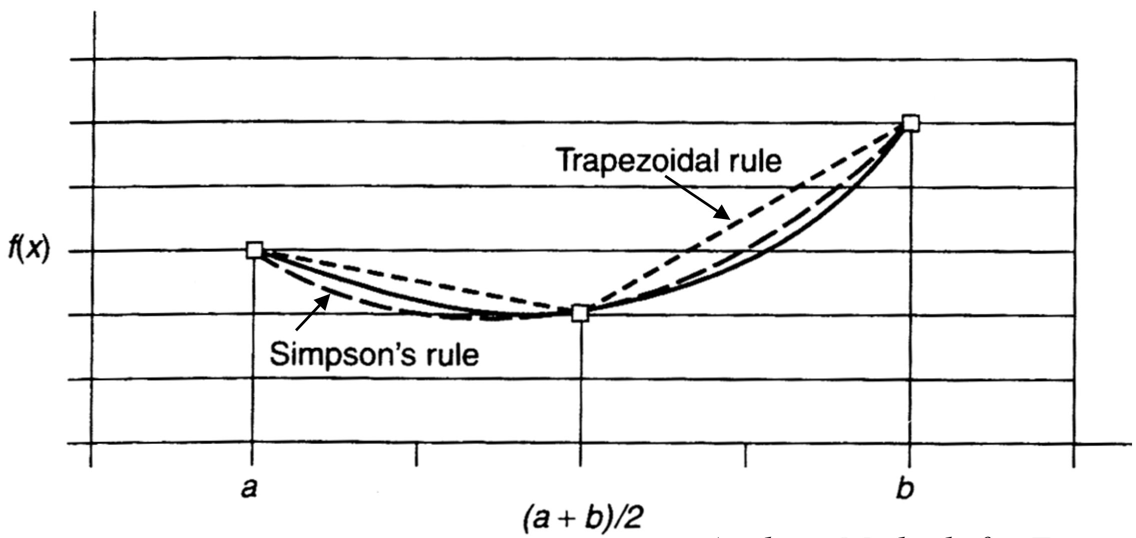
Numerical Integration

Simpson's Rule:

$$\int_{x_1}^{x_N} f(x)\,dx \approx \sum_{i=1,\,3,\,5}^{N-2} \frac{x_{i+2} - x_i}{2} \, \frac{f(x_{i+2}) + 4f(x_{i+1}) + f(x_i)}{3}$$

What is the basis of this formula?

⇨ each point fit by "quadratic" Lagrange polynomials



Analysis Methods for Engineers, Ayyub and McCuen

Numerical Integration

Simpson's Rule:

$$\int_{x_1}^{x_N} f(x)\,dx \;\approx\; \sum_{i=1,\;3,\;5}^{N-2} \frac{x_{i+2} - x_i}{2}\;\frac{f(x_{i+2}) + 4f(x_{i+1}) + f(x_i)}{3}$$

What is the basis of this formula?

⇨ each point fit by "quadratic" Lagrange polynomials

See pages 187 to 190 of *Numerical Analysis*, Burden and Faires,
for a derivation of Simpson's Rule
in terms of Quadratic Lagrange Polynomials

Analysis Methods for Engineers, Ayyub and McCuen

Numerical Integration

Simpson's Rule:

$$\int_{x_1}^{x_N} f(x)\,dx \approx \sum_{i=1,\,3,\,5}^{N-2} \frac{x_{i+2} - x_i}{2} \frac{f(x_{i+2}) + 4f(x_{i+1}) + f(x_i)}{3}$$

Error order d^4f/dx^4: i.e., fourth derivative of function evaluated at some place in the interval

Hence, Simpson's rule is exact for what order polynomial?

Numerical Integration

Boole's Rule (aka as Bode's rule):

$$\int_{x_1}^{x_N} f(x)\, dx \approx$$

$$\sum_{i=1,\ 5,\ 11,\ \ldots}^{N-4} \frac{x_{i+4} - x_i}{2} \; \frac{14 f(x_{i+4}) + 64 f(x_{i+3}) + 24 f(x_{i+2}) + 64 f(x_{i+1}) + 14 f(x_i)}{45}$$

Error order $d^6f(x)/dx^6$: i.e., sixth derivative of function evaluated at some place in the interval

Hence, Boole's rule is exact for what order polynomial?

Numerical Integration

Gaussian Quadrature:

$$\int_a^b f(x)\,dx = \int_{-1}^{1} f(g(y))\,\frac{dx}{dy}\,dy \approx \frac{1}{2}(b-a)\sum_{i=1}^{n} c_i f(g(y_i))$$

$y_1, y_2, \ldots y_n$ **nodes** are not uniformly spaced
$c_1, c_2, \ldots c_n$ **Gauss coefficients** are determined once ***n*** is specified

Note:

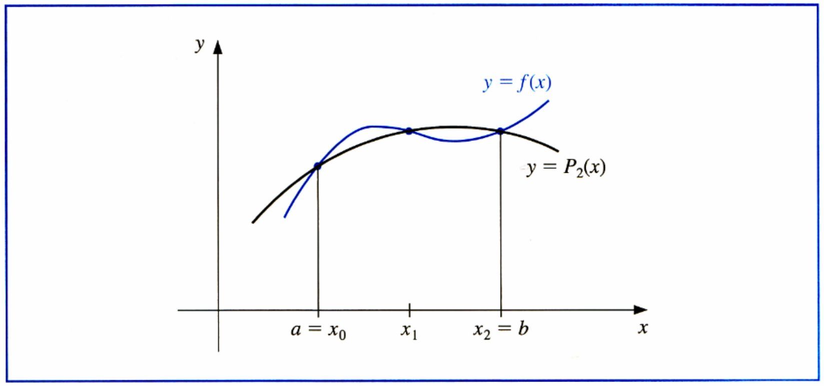
$$\int_{-1}^{1} f(y)\,dy \approx f\left(\frac{-\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right)$$

produces exact result for polynomials of degree 3 or less

Nice descriptions of theory at	http://en.wikipedia.org/wiki/Gaussian_quadrature
and	http://www.efunda.com/math/num_integration/num_int_gauss.cfm

Numerical Integration: Derivation of Simpson's rule, page 1

Figure 4.4



Therefore,

$$\int_a^b f(x)\,dx = \int_{x_0}^{x_2} \left[\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) \right.$$

$$\left. + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2) \right] dx$$

$$+ \int_{x_0}^{x_2} \frac{(x-x_0)(x-x_1)(x-x_2)}{6} f^{(3)}(\xi(x))\,dx.$$

Deriving Simpson's rule in this manner, however, provides only an $O(h^4)$ error term involving $f^{(3)}$. By approaching the problem in another way, a higher-order term involving $f^{(4)}$ can be derived.

To illustrate this alternative formula, suppose that f is expanded in the third Taylor polynomial about x_1. Then for each x in $[x_0, x_2]$, a number $\xi(x)$ in (x_0, x_2) exists with

$$f(x) = f(x_1) + f'(x_1)(x-x_1) + \frac{f''(x_1)}{2}(x-x_1)^2 + \frac{f'''(x_1)}{6}(x-x_1)^3 + \frac{f^{(4)}(\xi(x))}{24}(x-x_1)^4$$

and

$$\int_{x_0}^{x_2} f(x)\,dx = \left[f(x_1)(x-x_0) + \frac{f'(x_1)}{2}(x-x_1)^2 + \frac{f''(x_1)}{6}(x-x_1)^3 \right.$$

$$\left. + \frac{f'''(x_1)}{24}(x-x_1)^4 \right]_{x_0}^{x_2} + \frac{1}{24}\int_{x_0}^{x_2} f^{(4)}(\xi(x))(x-x_1)^4\,dx. \qquad (4.22)$$

R. L. Burden and J. D. Faires, Numerical Analysis, 8th edition

Numerical Integration: Derivation of Simpson's rule, page 2

Since $(x - x_1)^4$ is never negative on $[x_0, x_2]$, the Weighted Mean Value Theorem for Integrals implies that

$$\frac{1}{24}\int_{x_0}^{x_2} f^{(4)}(\xi(x))(x - x_1)^4\,dx = \frac{f^{(4)}(\xi_1)}{24}\int_{x_0}^{x_2}(x - x_1)^4\,dx = \frac{f^{(4)}(\xi_1)}{120}(x - x_1)^5\Big]_{x_0}^{x_2},$$

for some number ξ_1 in (x_0, x_2).

However, $h = x_2 - x_1 = x_1 - x_0$, so

$$(x_2 - x_1)^2 - (x_0 - x_1)^2 = (x_2 - x_1)^4 - (x_0 - x_1)^4 = 0,$$

whereas

$$(x_2 - x_1)^3 - (x_0 - x_1)^3 = 2h^3 \quad \text{and} \quad (x_2 - x_1)^5 - (x_0 - x_1)^5 = 2h^5.$$

Consequently, Eq. (4.22) can be rewritten as

$$\int_{x_0}^{x_2} f(x)\,dx = 2hf(x_1) + \frac{h^3}{3}f''(x_1) + \frac{f^{(4)}(\xi_1)}{60}h^5.$$

If we now replace $f''(x_1)$ by the approximation given in Eq. (4.9) of Section 4.1, we have

$$\int_{x_0}^{x_2} f(x)\,dx = 2hf(x_1) + \frac{h^3}{3}\left\{\frac{1}{h^2}[f(x_0) - 2f(x_1) + f(x_2)] - \frac{h^2}{12}f^{(4)}(\xi_2)\right\} + \frac{f^{(4)}(\xi_1)}{60}h^5$$

$$= \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{12}\left[\frac{1}{3}f^{(4)}(\xi_2) - \frac{1}{5}f^{(4)}(\xi_1)\right].$$

It can be shown by alternative methods (see Exercise 24) that the values ξ_1 and ξ_2 in this expression can be replaced by a common value ξ in (x_0, x_2). This gives Simpson's rule.

Thomas Simpson (1710–1761) was a self-taught mathematician who supported himself during his early years as a weaver. His primary interest was probability theory, although in 1750 he published a two-volume calculus book entitled *The Doctrine and Application of Fluxions*.

Simpson's Rule

$$\int_{x_0}^{x_2} f(x)\,dx = \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{90}f^{(4)}(\xi).$$

Since the error term involves the fourth derivative of f, Simpson's rule gives exact results when applied to any polynomial of degree three or less.

R. L. Burden and J. D. Faires, Numerical Analysis, 8th edition

Numerical Integration: Derivation of Simpson's rule, page 3

Example 1 The Trapezoidal rule for a function f on the interval [0, 2] is

$$\int_0^2 f(x)\,dx \approx f(0) + f(2),$$

and Simpson's rule for f on [0,2] is

$$\int_0^2 f(x)\,dx \approx \frac{1}{3}[f(0) + 4f(1) + f(2)].$$

The results to three places for some elementary functions are summarized in Table 4.7. Notice that in each instance Simpson's rule is significantly better. ■

R. L. Burden and J. D. Faires, Numerical Analysis, 8th edition