Towards assimilation of ExoMars TGO ACS observations into the LMD Mars GCM

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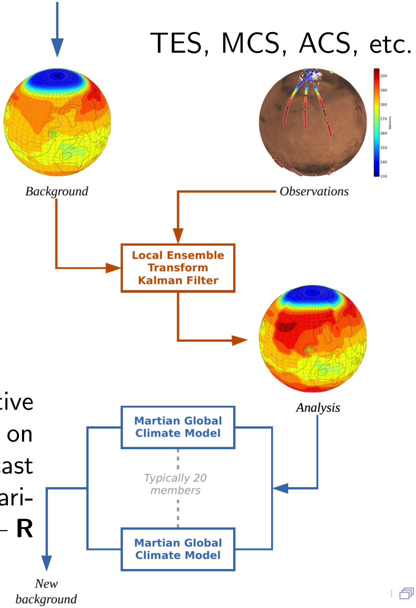
LMD data assimilation scheme for Mars

LMD Mars General Circulation Model

LETKF: Local Ensemble Transform Kalman Filter. Ensemble of 16 members estimates background mean $\bar{\mathbf{x}}^{\mathrm{b}}$ and error covariance $\mathbf{P}$.

Covariance inflation:

$\mathbf{P}$ increased by adaptive scalar factor based on comparison of forecast errors with error covariances $\langle \mathbf{d}\mathbf{d}^{\mathbf{T}} \rangle = \mathbf{H}\mathbf{P}\mathbf{H}^{\mathbf{T}} + \mathbf{R}$ (Miyoshi, 2011)



Some unobserved variables updated assuming same covariances and using known correlations (e.g. SW heating $\sim$ dust)

Always: $T \rightarrow T$

$T \rightarrow p_s, u, v$

Optional:

$T,\ q_{\mathrm{dust}} \rightarrow q_{\mathrm{dust}}$

$q_{\mathrm{ice}} \rightarrow q_{\mathrm{ice}}, q_{\mathrm{vap}}$

Current:

$T \rightarrow T, q_{\mathrm{dust}}$

No $q_{\mathrm{ice}},\ q_{\mathrm{vap}}$

[Navarro, 2016]

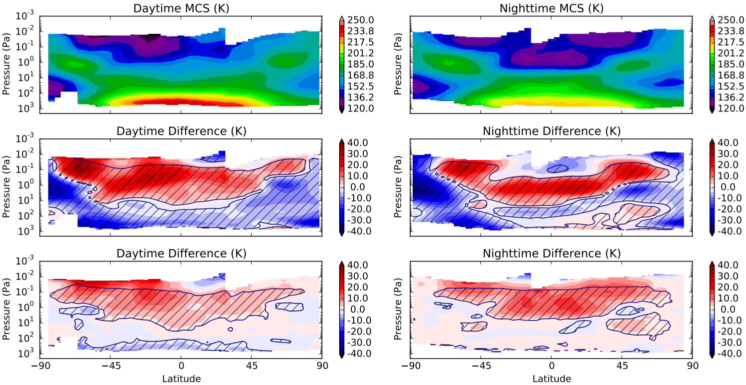
Temperature assimilation

Zonal mean temperature vs. MCS observations, MY29 $L_s = 165 - 170$

MCS 5-L_s binned observations

Free run
No assimilation

T assimilation
$T \rightarrow T, q_{\mathrm{dust}}$
6 hour cycle



Assimilation reduces distance between model temperatures and observations, particularly in lower atmosphere.

Effect of assimilation cycle length on temperature

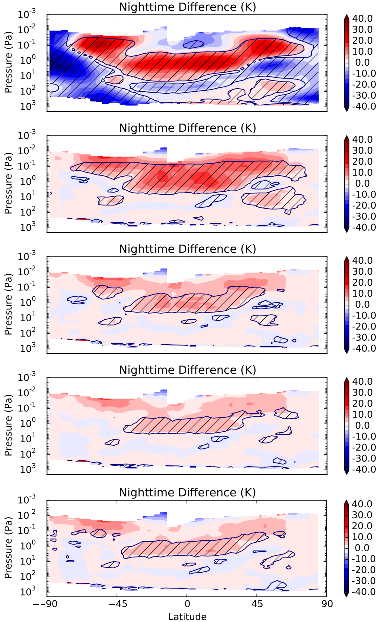
Free run
No assimilation

6 hour cycle

3 hour cycle

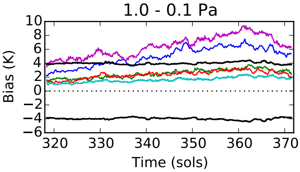
2 hour cycle

1 hour cycle

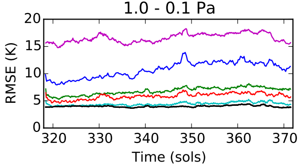


[Zonal sections averaged over $L_s = 165 - 170^{\circ}$]

Bias



RMSE

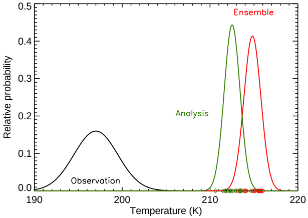


Zhao et al. (2015): Cycle <6 hours removes spurious forcing of semidiurnal tide

Error statistics stay closer to linear growth and so may remain Gaussian

Challenges for Mars ensemble-based data assimilation

Ensemble, observations diverge as ensemble converges (unlike Earth)

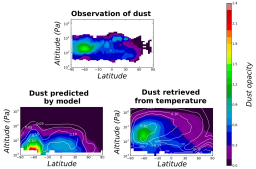


Dust / water ice hard to assimilate with temperature: all are inter-dependent

→ Observed q_{dust}, q_{ice} can easily fall outside ensemble when obs or whole ensemble = 0.

→ Ensemble aerosol uncertainty distributions are non-Gaussian.

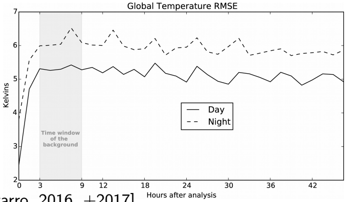
→ Observed dust structures may not be reproducible by model, so forecast step removes them.



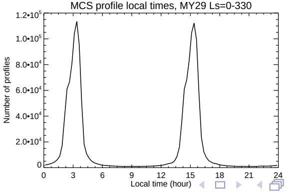
→ Water ice needs model-consistent dust concentration as condensation nuclei, otherwise forecast step will adjust one or the other.

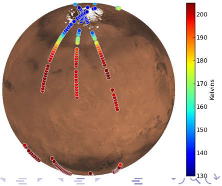
→ Direction of causality connecting changes in water ice and temperature is ambiguous.

Ensemble, observations diverge quickly once assimilation stops



Observations always at same local time of day (until TGO): 3h, 15h



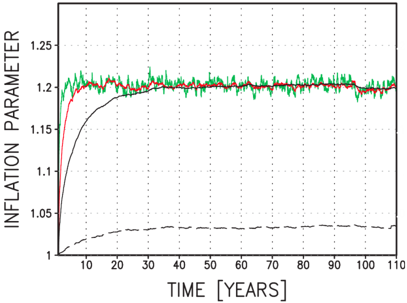


[Navarro, 2016, +2017]

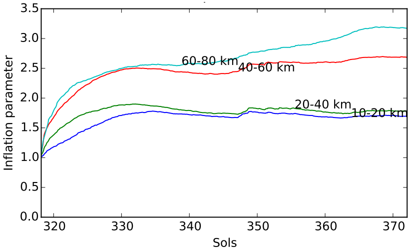
What is un-Earthlike — (1) Covariance inflation

Reminder (Miyoshi, 2011):
Multiply background error variance at observations by α_i
$\langle \mathbf{dd}^\mathbf{T} \rangle = \alpha_i \mathbf{HPH}^\mathbf{T} + \mathbf{R}$ where $\mathbf{d} = \mathbf{y} - H(\mathbf{x}^\mathbf{b})$. KF updates α_i.

Imperfect Lorenz-96 [Miyoshi, 2011]



Mars example
($L_s = 150 - 180^\circ$ temperature)



Inflation parameter is $\gg 1$. Will occur when ensemble SD is underestimated, but also when bias $\gg$ observational error.

What is un-Earthlike — (2) Chaos and bias

Mars' atmosphere is not always chaotic

Breeding vector growth rates

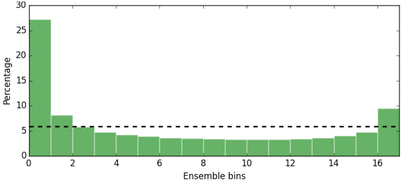
Month	Time of year	Mean daily growth rate
1	Northern mid-spring	−0.0197
2		−0.0495
3		−0.00308
4	Northern mid-summer	−0.0307
5		−0.0494
6		−0.0363
7	Northern mid-autumn	−0.0376
8		0.130
9		0.262
10	Northern mid-winter	0.330
11		0.126
12		0.140

[Newman et al., 2004]

Always +ve for Earth

Many observations fall outside ensemble

Rank histogram
($L_s = 150 - 180°$, temperature)



~35% observations outside

Bias $+0.4\sigma$, spread 0.5σ [Hamill, 2001]

On Mars, model–obs distance can become dominated by model error. Ensemble shrinks over time at certain times of year. Can't be alleviated by chaos expanding ensemble to fill state space.

Correction steps in ensemble data assimilation

E.g. Earth atmosphere/oceans, oil industry reservoir modelling

- (1) Estimate, remove bias (forecast mean - observations $\neq 0$)
- (2) Correct for model errors (additional matrix "big **Q**" in background error covariance)
- (3) Covariance inflation

Bias correction (method from Dee & Da Silva, 1998):

- "Forecast bias" = "Non-zero mean forecast error"
- If forecast is biased, assigning more weight to observations will reduce bias, but analysis will be noisier.
- Unbiased Kalman filter:

$$\tilde{\mathbf{x}}^{\mathrm{a}} = \tilde{\mathbf{x}}^{\mathrm{b}} + \mathbf{K}(\tilde{\mathbf{y}}^{\mathrm{o}} - H[\tilde{\mathbf{x}}^{\mathrm{b}}]) \qquad \mathbf{K} = \mathbf{P}\mathbf{H}^{\mathbf{T}}[\mathbf{H}\mathbf{P}\mathbf{H}^{\mathbf{T}} + \mathbf{R}]^{-1}$$

- Where unbiased quantities are
  $\tilde{\mathbf{x}}^{\mathrm{a}} = \mathbf{x}^{\mathrm{a}} - \mathbf{b}^{\mathrm{a}} \qquad \tilde{\mathbf{y}}^{\mathrm{o}} = \mathbf{y}^{\mathrm{o}} - \mathbf{b}^{\mathrm{o}} \qquad \tilde{\mathbf{x}}^{\mathrm{b}} = \mathbf{x}^{\mathrm{b}} - \mathbf{b}^{\mathrm{b}}$
- Plug these in and, assuming observation operator is linear:

$$\mathbf{x}^{\mathrm{a}} = \mathbf{x}^{\mathrm{b}} + \mathbf{K}[\mathbf{y}^{\mathrm{o}} - \mathbf{H}\mathbf{x}^{\mathrm{b}}] \qquad \mathbf{b}^{\mathrm{a}} = \mathbf{b}^{\mathrm{b}} + \mathbf{K}[\mathbf{b}^{\mathrm{o}} - \mathbf{H}\mathbf{b}^{\mathrm{b}}]$$

Accounting for model error

Additive inflation ("big Q")

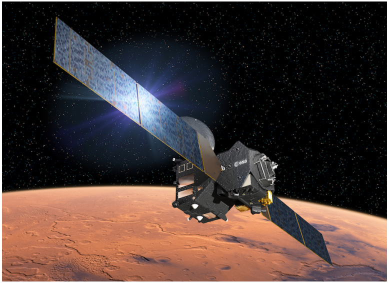
- Parametrizes model errors by adding random perturbations with a certain covariance structure to each ensemble member.
- $\mathbf{x}_k^f = \mathbf{x}_{e(k)}^f + r\mathbf{q}_k$ with $\bar{\mathbf{q}}_k = 0$, r constant tuneable parameter.
- Background error covariance increases by $\mathbf{Q} = r^2 \langle \mathbf{q}_k \mathbf{q}_k^T \rangle$ but in a physically sensible way.
- Li+ (2009) [Earth atmosphere]: $\mathbf{q}_k$ are randomly selected 6h tendencies in NCEP reanalyses (i.e. the selection is random, not the field). Geostrophically balanced.
- Lang+ (2017) [Solar wind]: "$\mathbf{Q}$ ... *contains the relevant MHD balances to perturb the ensemble with a model error term*"

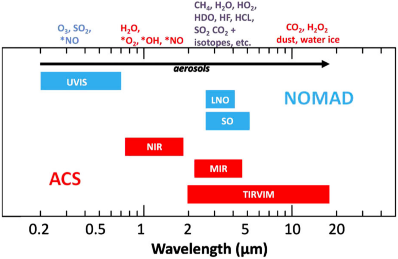
Parameter ensemble

- Simplest form: Assign different values of unknown parameters to different ensemble members (e.g. Greybush et al. 2012 for dust opacities)

ESA/Roscosmos ExoMars Trace Gas Orbiter

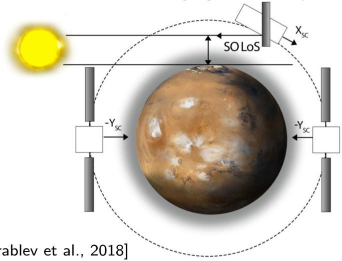
Main goal: To search for rarified gases such as methane





Inserted into Mars orbit 19 October 2016.
Reached final orbit 7 April 2018.

TGO viewing geometry



Instruments:
ACS (3 infrared spectrometers),
CASSIS (stereo visible imaging camera),
FREND (neutron detector — subsurface),
NOMAD (3 infrared/UV spectrometers)

[Korablev et al., 2018]

Towards assimilation of ACS data

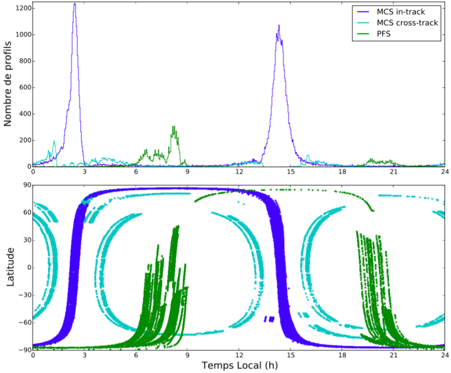
Thermal infrared channel (TIRVIM). Retrievals at LMD by Sandrine.

Initially: Atmospheric temperature profiles

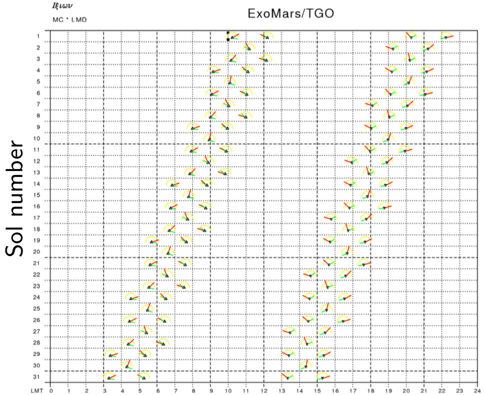
Potentially: Surface temperatures, column dust opacity, column ice opacity

Local times vs MCS:

MCS/PFS local times



ACS local times at 45°N / 0°E



Local time

[Navarro, 2016]

Observation operator for TIRVIM $\left(\mathbf{x}^{\mathrm{a}} = \mathbf{x}^{\mathrm{b}} + \mathbf{K}(\mathbf{y}^{\mathrm{o}} - H[\mathbf{x}^{\mathrm{b}}])\right)$

What would a retrieval (of e.g. T) look like if TIRVIM observed the background $\mathbf{x}^{\mathrm{b}}$?

- This is the correct comparison with retrieved observations $\mathbf{y}^{\mathrm{o}}$.
- Earlier work with MCS used (naïve, but simpler) linear interpolation to observation points.
- [Alternative — assimilate radiances directly]

Correct form is observation- and instrument-specific.
Our TIRVIM assimilation scheme uses two steps:

- Interpolate background to retrieval position and pressures, as before (linear in $\mathbf{x}$, t)
- Use averaging kernels to retrieve what ACS would see:

$$\hat{\mathbf{x}} = \mathbf{x}^{\mathrm{p}} + \mathbf{A}(\mathbf{x}^{\mathrm{b}} - \mathbf{x}^{\mathrm{p}})$$

(Rodgers & Connor, 2003) Prior $\mathbf{x}^{\mathrm{p}}$ and averaging kernels $\mathbf{A}$ are the same as for retrieval used to create observations $\mathbf{y}^{\mathrm{o}}$.

Current goals

Improving assimilation scheme

- Work out what's going on with aerosols
- Explicit correction of forecast biases
- Ensemble of poorly constrained parameters

Assimilating ACS observations

- Start working with calibrated observations
- Set up pipeline to assimilate as new retrievals come in
- Add T_{surf}, dust and ice column-integrated quantities to assimilation
- Co-assimilation of ACS and MCS observations
- See EPSC in September for progress...!

Talking points

Mars atmosphere fundamentally different from Earth's (sometimes non-chaotic)

Ensemble schemes can struggle with this

Help and ideas are available from other fields, where non-chaotic systems are more common

These three correction steps are well-established in more fully-developed ensemble data assimilation:

- (1) Estimate and remove bias
- (2) Correct for model errors ("big $\mathbf{Q}$")
- (3) Covariance inflation