Soil Moisture
Active Passive
Mission
SMAP
Cal/Val Workshop #4
November 5-7, 2013

L4_SM
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John Kimball (U. Montana)
Outline

1) Motivation and requirements
2) Calibration and validation approach and activities
3) Validation of prototype L4_SM products
   - Rehearsal Phase 1 – model-only prototype product
   - Prototype product based on SMOS assimilation
Key limitations of SMAP observations

SMAP observations:

1) are sensitive to moisture and temperature only in a 5 cm surface layer (and only if less than 5 kg/m² vegetation),
2) have limited coverage in time and space, and
3) are subject to measurement errors.

Need root-zone soil moisture for many applications of interest to SMAP.
SMAP Level 4 soil moisture product

L4_SM Product:
Assimilating SMAP data into a land model driven with observation-based forcings yields:
– a root-zone moisture product (reflecting SMAP data), and
– a complete and consistent estimate of soil moisture & related fields.

L4_SM output includes
• global,
• 3-hourly,
• 9 km
estimates of surface (0-5 cm) and root zone (0-100 cm) soil moisture.

Surface meteorology

SMAP observations

Data Assimilation

Land model

L4_SM Product: Surface and root-zone soil moisture

Applications Users
Motivated by the SMAP Level 1 Science Requirements, the

**L4_SM surface (0-5 cm) and root zone (0-100 cm) soil moisture** estimates will be validated to an [ubRMSE requirement of 0.04 m³m⁻³.](ubRMSE = RMSE after removal of long-term mean bias.)

[Identical to L2 soil moisture product validation and excluding regions of snow and ice, frozen ground, mountainous topography, open water, urban areas, and vegetation with water content greater than 5 kg m⁻².]

**Research outputs** (surface meteorological forcing fields, land surface fluxes, soil temperature and snow states, runoff, and ensemble-based error estimates) will be evaluated on a best effort basis.
1) Motivation and requirements
2) Calibration and validation approach and activities
3) Validation of prototype L4_SM products
   - Rehearsal Phase 1 – model-only prototype product
   - Prototype product based on SMOS assimilation
<table>
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<th>Data</th>
<th>Importance</th>
<th>Metric</th>
</tr>
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<td>Core Sites</td>
<td>Observed grid cell average values</td>
<td>Primary</td>
<td>RMSE, bias, correlation</td>
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<td>(time-continuous)</td>
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<td>Sparse Networks</td>
<td>Observed values</td>
<td>Primary</td>
<td>Correlation, RMSE, bias</td>
</tr>
<tr>
<td></td>
<td>(time-continuous)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Satellite Products</td>
<td>Orbit-based match-ups (SMOS, ASCAT, ...)</td>
<td>Secondary:</td>
<td>Correlation, RMSE, bias</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Pending cont’d operation</td>
<td></td>
</tr>
<tr>
<td>Model Products</td>
<td>Global modeling and assimilation systems</td>
<td>Primary</td>
<td>RMSE, bias, correlation, assim. diagn.</td>
</tr>
<tr>
<td></td>
<td>(ECMWF, NCEP, ...)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Field Experiments</td>
<td>Detailed estimates for a very limited set</td>
<td>Secondary</td>
<td>RMSE, bias, correlation</td>
</tr>
<tr>
<td></td>
<td>of conditions</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Will be used to verify “0.04 m$^3$m$^{-3}$” requirement
Cal/Val activities to date:

• Calibrating modeling and assimilation system:
  – Soil parameters.
  – Microwave radiative transfer (tau-omega) model parameters.
  – Model and observation error parameters.
• Participated in Cal/Val Rehearsal Phase 1.
• Validating L4_SM system driven with SMOS Tb obs.
1) Motivation and requirements
2) Calibration and validation approach and activities
3) Validation of prototype L4_SM products
   - Rehearsal Phase 1 – model-only prototype product
   - Prototype product based on SMOS assimilation
Validation at core-site reference pixels (surface)

Average: $\text{ubRMSE}=0.041 \text{ m}^3/\text{m}^3$

- 16010901 (Walnut Gulch): $\text{ubRMSE}=0.029 \text{ m}^3/\text{m}^3$
- 16040901 (Little River): $\text{ubRMSE}=0.046 \text{ m}^3/\text{m}^3$
- 16040902 (Little River): $\text{ubRMSE}=0.037 \text{ m}^3/\text{m}^3$
- 25010901 (Tonzi Ranch): $\text{ubRMSE}=0.020 \text{ m}^3/\text{m}^3$
- 41010902 (Valencia): $\text{ubRMSE}=0.036 \text{ m}^3/\text{m}^3$
- 16070901 (South Fork): $\text{ubRMSE}=0.076 \text{ m}^3/\text{m}^3$

Red: Core-site in situ measurements
Black: L4_SM (model-only prototype, no data assimilation)

Special thanks to A. Colliander & M. Cosh!
**Validation at core-site reference pixels (surface)**

Additional metrics are also reported.

<table>
<thead>
<tr>
<th>Site</th>
<th>RefPix</th>
<th>ubRMSE</th>
<th>Bias</th>
<th>RMSE</th>
<th>R</th>
<th>Site name</th>
</tr>
</thead>
<tbody>
<tr>
<td>1601</td>
<td>0901</td>
<td>0.029</td>
<td>0.056</td>
<td>0.065</td>
<td>0.652</td>
<td>Walnut Gulch</td>
</tr>
<tr>
<td>1604</td>
<td>0901</td>
<td>0.046</td>
<td>0.023</td>
<td>0.041</td>
<td>0.456</td>
<td>Little River</td>
</tr>
<tr>
<td>1604</td>
<td>0902</td>
<td>0.037</td>
<td>-0.004</td>
<td>0.044</td>
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<tr>
<td>2501</td>
<td>0901</td>
<td>0.020</td>
<td>0.074</td>
<td>0.073</td>
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</tr>
<tr>
<td>1607</td>
<td>0901</td>
<td>0.086</td>
<td>0.072</td>
<td>0.101</td>
<td>0.627</td>
<td>South Fork</td>
</tr>
<tr>
<td>4101</td>
<td>0902</td>
<td>0.036</td>
<td>0.098</td>
<td>0.096</td>
<td>0.659</td>
<td>Valencia</td>
</tr>
</tbody>
</table>

**Average**

0.044 0.053 0.070 0.589 **Average**

(L4_SM is model-only prototype, no data assimilation)
Validation at core-site reference pixels (root zone)

Red: Core-site in situ measurements [avg. of 5, 10, 20, and 50cm obs]
Black: L4_SM (model-only prototype)

Special thanks to A. Colliander & M. Cosh!
Outline

1) Motivation and requirements
2) Calibration and validation approach and activities
3) Validation of prototype L4_SM products
   - Rehearsal Phase 1 – model-only prototype product
   - Prototype product based on SMOS assimilation
• **Assimilate SMOS Tb** (7 angles, 36 km, 6 am/pm, H- and V-pol)
• MERRA surface meteorology
• CPCU daily 0.5 deg precipitation corrections
• 9 km EASEv2 Catchment model resolution
• Calibrated microwave RTM parameters
• Mean-adjustment of SMOS observations prior to assimilation
L4_SM_SMOS: Cal/Val (core) sites

Little Washita

Surface

Root zone

Green: In situ
Red: L4_SM_SMOS
Black: Model only
L4_SM_SMOS: Cal/Val (core) sites

- **ubRMSE** reduced to less than 0.04 m³/m³.
- **(Anomaly) correlation** significantly increased (except RC).
- **Bias** reduced.

**Bias [m³/m³]**

- Black: Model only
- Gray: L4_SM_SMOS

**ubRMSE [m³/m³]**

**Anom R [-]**

Apr 2010 – Mar 2011
**L4_SM_SMOS: Sparse networks**

<table>
<thead>
<tr>
<th>SCAN/SNOTEL</th>
<th>USCRN</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Surface soil moisture</strong></td>
<td><strong>Surface soil moisture</strong></td>
</tr>
<tr>
<td>ubRMSE=0.056 m³/m³</td>
<td>ubRMSE=0.052 m³/m³</td>
</tr>
<tr>
<td>N=183</td>
<td>N=77</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Root zone soil moisture</strong></th>
<th><strong>Root zone soil moisture</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>ubRMSE=0.046 m³/m³</td>
<td>ubRMSE=0.041 m³/m³</td>
</tr>
<tr>
<td>N=183</td>
<td>N=77</td>
</tr>
</tbody>
</table>
Root zone soil moisture

ubRMSE=0.04 m³/m³
N=38

COSMOS

L4_SM_SMOS: Sparse networks
Thank you for your attention!
EXTRA SLIDES
Cal/Val extras
Diagnostics of filter performance

Filter update:  \( x^+ = x^- + K(y - x^-) \)
\[ K = P \frac{1}{P + R} = \text{Kalman gain} \]

Diagnostic:  \( \mathbb{E}[(y - x^-)(y - x^-)^T] = P + R \)

\( x^- = \text{model forecast} \)
\( x^+ = \text{“analysis”} \)
\( y = \text{observation} \)

Innovations \( \equiv \text{obs} - \text{model prediction} \)
(internal diagnostic)

State err cov + obs err cov
(controlled by inputs)

Innovations diagnostics are ALWAYS available within assimilation system.

- Mean of innovations should equal zero. **Otherwise have bias!**
- Normalize innovations with \( \sqrt{P+R} \) \( \rightarrow \) std-dev should equal one.
  **Otherwise (input) model and obs error parameters are inconsistent!**

Example:
1) Bias.
2) Input uncertainties too small.
Normalized innovations histograms suggest some over-estimation of the input error variances (of model and/or observations).
**L4_SM_SMOS: Innovations and increments**

**Innovations (36 km observation space)**
- Mean of innovations
  - $\text{avg} = 0.4$ K, $\text{avg abs} = 0.7$ K
- Stdv of normalized innovations
  - $\text{avg} = 0.82$

**Innovations (9 km model space)**
- Stdv of surface excess incr.
  - $\text{avg} = 0.6$ mm
- Stdv of root zone excess incr.
  - $\text{avg} = 2.7$ mm
- Number of increments per day
  - (avg: ~1 every other day)

**Apr 2010 – Mar 2013**
**L4_SM_SMOS: Ensemble error estimates**

**Tb ensemble std-dev (36 km obs. space)**

- **Mean forecast** error std-dev
  - avg = 1.5 K

- **Mean analysis** error std-dev
  - avg = 0.83 K

- **Mean analysis/forecast** error std-dev (avg = 0.67)

**Increments (9 km model space)**

- Stdv of **surface** excess incr.
  - avg = 0.6 mm

- Stdv of **root zone** excess incr.
  - avg = 2.7 mm

**Tb forecast errors and soil moisture increments are small over densely vegetated regions.**

(Soil moisture ensemble spread was not written out and remains to be evaluated.)
Impact of CPCU on soil moisture skill: CalVal sites

Withholding CPCU precipitation corrections simulates conditions in poorly observed regions. Improvements from Tb assimilations are somewhat greater without CPCU corrections. ubRMSE still close to 0.04 m³/m³.
Impact of CPCU on soil moisture skill improvement: SCAN/Snotel

With CPCU precipitation

ΔanomR = anomR(assim) − anomR(model)

Surface soil moisture

ΔanomR = 0.08
N=161

ΔanomR = 0.10
N=161

Root-Zone soil moisture

ΔanomR = 0.19
N=161

Without CPCU precipitation

ΔanomR = 0.16
N=161

ΔanomR = 0.19
N=161

36 km model

Greater improvements in terms of anomaly R without CPCU corrections.
Post-launch, emphasis is on validation of the L4_SM data product.

Post-launch validation:
- See earlier slides on validation requirements, data resources, and approach.
- Can ingest IOC and Cal/Val phase L1 and L2 brightness temperature observations, but poor quality data likely eliminated during L4_SM internal QC.

Refine algorithm calibration as needed (SMOS → SMAP):
- Re-calibrate microwave radiative transfer model parameters to SMAP Tb.
- Re-derive scaling parameters for SMAP-based system.
- Adjust model and observation error standard deviations in response to SMAP-based observation-minus-forecast residuals.
- Re-calibrate F/T analysis using SMAP F/T observations.

Operational monitoring:
- QC/QA (e.g., checks against range thresholds)
- Assimilation diagnostics
**L4_SM Cal/Val Schedule**

- SMOS-based **L4_SM calibration** (on-going).
- Science algorithm software **Delivery 5** (Feb 2014).
- SMAP **Cal/Val Rehearsal Phase 2** (May 2014).
- SMAP **launch** (Oct 2014) and IOC (Winter 2014/15); initiation of SMAP operations and L4_SM production.
- **Post-launch Cal/Val activities** (Feb 2015-Jan 2016).
- L4_SM **Beta Product release** to NSIDC (6 months after IOC; Aug 2015).
- L4_SM **Stage I Validated Product release** to NSIDC (12 months after IOC; Feb 2016).
- Release of post-launch **Cal/Val report** (Feb 2016).
Algorithm development extras
Consider an arbitrary point in the catchment:

- **Integrate:** yellow area = moisture deficit, $D$, at this point.
- equilibrium profile
- water table

Now integrate $D$ across the catchment:

\[
\text{CATDEF} = \frac{1}{A} \int_A D \, dA
\]

= the average amount of water, per m$^2$, that must be added to the catchment to bring it to complete saturation, assuming equilibrium profiles.

**“Catchment Deficit” variable**

**“Root Zone Excess” and “Surface Excess” variables: the view at a point**

- SRFEXC: amount by which surface moisture exceeds equil. in root zone
- RZEXC: amount by which root zone moisture exceeds equil.

**Diffusion calculation**

Functions relating time scales of diffusion to the moisture variables are pre-computed from Richard’s equation calculations at high vertical resolution. The time scales for diffusion between RZEXC and CATDEF reflect net diffusion over a spatially distributed set (across the catchment) of independent columns.

*Koster et al. (2000) Ducharne et al. (2000)*
### L4_SM data product overview

#### SMAP inputs

- **Brightness temperature**
  - (L1C_TB, 36 km)
  - (L2_SM_AP, 9 km)

- **Freeze-thaw state**
  - (L2_SM_A, 3 km)

#### Ancillary data inputs

- Land model parameters
- Surface meteorology (incl. observation-corrected precip)
- Land assimilation parameters

#### L4_SM product

- 9 km, 3-hourly global output with 7-day latency

- **Surface soil moisture** (≡ top 5 cm)
- **Root zone soil moisture** (≡ top 1 m)

**Research output**

- surface and soil temperatures *(input to L4_C)*
- sensible, latent, and ground heat flux
- runoff, baseflow, snowmelt
- surface meteorological forcings (air temperature, precipitation, …) *[ancillary]*
- **error estimates** (generated by assimilation system)
- assimilation diagnostics (observations-minus-forecast residuals, increments)
L4_SM data product overview (2)

- L4_SM provides a global product → **no exclusion masks** (besides QC of assimilated observations).
- L4_SM provides quantitative information about snow, soil temperature, etc → **binary flags not needed** in most cases.
- “aup” Collection includes error estimates (ensemble spread) and assimilation diagnostics (observations-minus-forecast residuals, increments)
Baseline algorithm:
- Customized version of NASA GEOS-5 Land Data Assimilation System
  - 3d ensemble Kalman filter: *spatial extrapolation, interpolation, and disaggregation of assimilated observations*
  - Catchment land surface model with tau-omega microwave radiative transfer model
  - Observations-based precipitation
- No optional algorithms.
**L4_SM analysis overview**

**L4_SM LAND MODEL**
- FCST(t) 9 km → Model integration (forecast) → F/T FCST 9 km

**SMAP OBSERVATIONS**
- F/T OBS 3 km → Aggregate → 9 km

**Agree?**
- no → Freeze-thaw analysis: Update soil heat content
- yes → Frozen? (no) → Soil moisture analysis: Update soil moisture and soil heat content
- yes → No analysis

**ANA(t-1) 9 km**

**ANA(t) 9 km**
L4_SM soil moisture analysis

L4_SM LAND MODEL

- FCST(t) 9 km
  - TBH, TBV 9 km
  - Aggregate
    - 36 km
      - Clim. mean adjustment
        - 36 km

SMAP OBSERVATIONS

- 3d EnKF analysis
  - Innovations (OBS – FCST) 9 km, 36 km
    - Available?
      - no
        - TBH, TBV (L2_SM_AP) 9 km
        - Clim. mean adjustment
          - 9 km
          - Diff.
            - 9 km
      - yes
        - TBH, TBV (L1C_TB) 36 km
        - Clim. mean adjustment
          - 36 km

L4_SM soil moisture analysis (2)

Analyzed model states:

\[
\begin{pmatrix}
 x_1^- \\
 x_2^- \\
 \vdots \\
 x_{N9}^-
\end{pmatrix}
\]

where

\[
\begin{pmatrix}
 SRFEXC_FCST_j \\
 RZEXC_FCST_j \\
 CATDEF_FCST_j \\
 TC1_FCST_j \\
 TC2_FCST_j \\
 TC4_FCST_j \\
 GHT1_FCST_j
\end{pmatrix}
\]

Soil moisture prognostic variables.

Surface temperature and top-layer soil temperature prognostic variables.

N9: # of 9 km grid cells incl. in soil moisture analysis.

j=1...N9

Subscripts for time and ensemble member omitted.
NOAA/CPC Unified Daily Gauge Data

- Provided on 0.5 deg grid with ~2-day latency
- Dense gauge networks from special CPC collections in US, Mexico, and S. America
- GTS gauge network elsewhere
- Daily reports available from ~17,000 stations
Precipitation corrections

**GEOS-5 (NWP)**
Hourly
0.25° x 0.3125°

**Rescale GEOS-5**
separately for each day and
0.25° x 0.3125° grid cell

**CPCU Gauges**
Daily
0.5° x 0.5°

**GEOS-5 + CPCU**
(hourly, 0.25° x 0.3125°)

For each day and each 0.25° x 0.3125° grid cell, the corrected GEOS-5 precipitation (almost) matches CPCU observations.
Satellite remote sensing of (surface) soil moisture

2009-present
L-band passive
40 km resolution
Interferometric & multi-angular

Launch: 2014
L-band active/passive
3-40 km resolution
Zero-order (tau-ω) microwave radiative transfer model

Key microwave parameters:

- Vegetation opacity (τ)
- Scattering albedo (ω)
- Soil roughness (h)

$T_{b,TOA}$
$T_{b,TOV}$

atmospheric contributions

attenuation by vegetation

θ
For some RTM parameter sets, GEOS-5 (model) Tb is strongly biased vs. SMOS observations.

Prescribed RTM parameters:
Lit1: SMAP Level2 ATBD
Lit2: LMEB literature
Lit3: ECMWF SMOS monitor

De Lannoy et al, 2013, doi: 10.1175/JHM-D-12-092.1
**L-band brightness temp.: SMOS vs. GEOS-5**

One-year mean [K]

**SMOS**

H-pol 42.5°  Jul 2010 – Jun 2011 (validation period)


**Calibrated parameters yield mostly unbiased long-term mean Tb.**

**Literature values for parameters yield strongly biased Tb.**

- **Lit1**
  - avg(|L|) = 42.0 K

- **Lit2**
  - avg(|L|) = 12.7 K

- **Lit3**
  - avg(|L|) = 24.6 K

- **CalD2**
  - avg(|L|) = 2.7 K
L-band brightness temp.: SMOS vs. GEOS-5

- H-pol 6 am vs. V-pol 6 am
- H-pol 6 pm vs. V-pol 6 pm
- Time (Jan 2010 – Oct 2012)
- Small bias: 6 am vs. 6 pm

#43
Some bias remains between observations and simulations. (e.g., due to errors in seasonal cycle of vegetation inputs, seasonal and diurnal errors in soil temperature inputs, imperfect observations, and/or imperfect calibration).

Adjust Tb observations such that their (3-year) mean value for each grid cell matches that of the simulated Tb. (separately for each day-of-year, after smoothing)

Example of residual biases after calibration of microwave RTM parameters (6 am, 40° inc angle, H-pol, June 2010 – May 2013)
L-band brightness temp.: SMOS (scaled) vs. GEOS-5

[a) H-pol 6 am  V-pol 6 am
   Time (Jan 2010 – Nov 2012)

[b) H-pol 6 pm  V-pol 6 pm
   Time (Jan 2010 – Nov 2012)
**Observation and model error parameters**

Input parameter settings evolved from soil moisture retrieval assimilation. **Algorithm calibration** primarily adjusts these parameters, based on validation metrics (see below).

Horizontal scale of distributed (3d) analysis: 1.25 deg (radius)

**Model forcing error parameters**

<table>
<thead>
<tr>
<th>Perturbation</th>
<th>Additive (A) or Multiplicative (M)?</th>
<th>Standard deviation</th>
<th>AR(1) time series correlation scale</th>
<th>Spatial correlation scale</th>
<th>Cross-correlation with perturbations in</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>P</td>
</tr>
<tr>
<td>Precipitation (P)</td>
<td>M</td>
<td>0.5</td>
<td>1 day</td>
<td>0.5 deg</td>
<td>1.0</td>
</tr>
<tr>
<td>Downward shortwave radiation (SW)</td>
<td>M</td>
<td>0.3</td>
<td>1 day</td>
<td>0.5 deg</td>
<td>-0.8</td>
</tr>
<tr>
<td>Downward longwave radiation (LW)</td>
<td>A</td>
<td>20 W m(^{-2})</td>
<td>1 day</td>
<td>0.5 deg</td>
<td>0.5</td>
</tr>
</tbody>
</table>

Observation error parameters (SMOS Tb)

- Standard deviation: 8 K
- (additive, uncorrelated in space and time)
### Observation and model error parameters

(Prognostics perturbations account for errors in model structure and model parameters.)

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</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Catdef</td>
</tr>
<tr>
<td>Catchment deficit (Catdef)</td>
<td>A</td>
<td>0.07 mm</td>
<td>3 h</td>
<td>0.5 deg</td>
<td>1.0</td>
</tr>
<tr>
<td>Surface excess (Srfexc)</td>
<td>A</td>
<td>0.04 mm</td>
<td>3 h</td>
<td>0.5 deg</td>
<td>0.0</td>
</tr>
<tr>
<td>Surface temperature (Tsurf)</td>
<td>A</td>
<td>0.2 K</td>
<td>3 h</td>
<td>0.5 deg</td>
<td>0.5</td>
</tr>
<tr>
<td>Top-layer soil heat content (Ght1)</td>
<td>A</td>
<td>500 J/m(^2)</td>
<td>3 h</td>
<td>0.5 deg</td>
<td>0.3</td>
</tr>
</tbody>
</table>
\[ \Delta \text{RMSE}^* \] [K]  
\begin{array}{cccccc}
<table>
<thead>
<tr>
<th>Max. classification error [%]</th>
<th>0</th>
<th>5</th>
<th>10</th>
<th>20</th>
<th>30</th>
</tr>
</thead>
<tbody>
<tr>
<td>T_{\text{skin}}</td>
<td>3.08</td>
<td>0.21</td>
<td>0.19</td>
<td>0.18</td>
<td>0.15</td>
</tr>
<tr>
<td>T_{\text{soil}}</td>
<td>1.97</td>
<td>0.06</td>
<td>0.05</td>
<td>0.04</td>
<td>0.01</td>
</tr>
</tbody>
</table>
\end{array}

*Excl. times & locations with T_{\text{air}} > 7^\circ \text{C} or T_{\text{air}} < -7^\circ \text{C}

\[ \Delta \text{RMSE} \text{ T}_{\text{skin}} = 0.15 \text{ K} \]

\[ \Delta \text{RMSE} \text{ T}_{\text{soil}}(5\text{cm}) = 0.01 \text{ K} \]

Minimal improvements with realistic classification errors.

Farhadi et al., 2013, in prep.