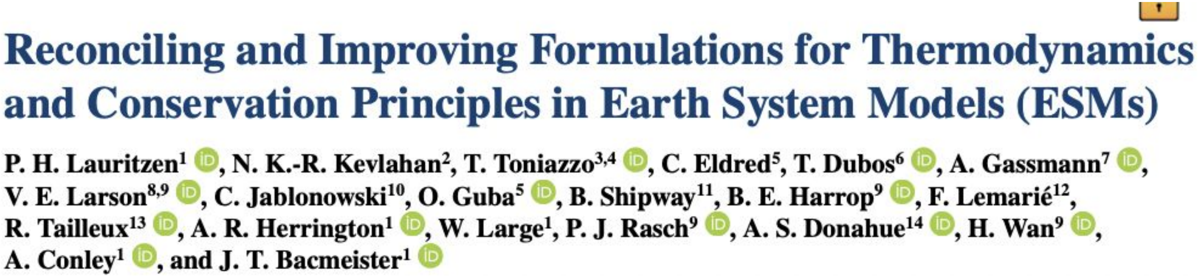
NATIONAL CENTER FOR ATMOSPHERIC RESEARCH

Coupling dynamics and physics is a science problem!



Reconciling and Improving Formulations for Thermodynamics and Conservation Principles in Earth System Models (ESMs)

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PDC22
4th Workshop on Physics-Dynamics Coupling in Weather & Climate Models

A Workshop in Honor and Memory of Markus Sebastian Gross
Princeton University, 1-3 June 2022

Featured as Editor's Highlight in Eos:
https://eos.org/editor-highlights/consistently-closing-the-energy-budget-in-earth-system-models

Paper link: https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2022MS003117
(warning: 83 pages)

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Towards an energy consistent coupling of the height-based Model for Prediction Across Scales Atmosphere (MPAS-A) dynamical core with the pressure-based Community Atmosphere Model (CAM) physics packages

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Presentation at Workshop on Modelling the Climate System at Ultra-High-Resolution

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Motivation

Most comprehensive physics packages, e.g., NCAR’s Community Atmosphere Model (CAM) physics,

- are formulated in hydrostatic pressure (/mass) coordinates and assume that pressure stays constant during physics updates (i.e. enthalpy conservation from 1st law of thermodynamics)
- only include dry air and water vapor in pressure/density
- used in coupled climate models are formulated for a closed total energy budget (closely related to *thermodynamic consistency*)

Many weather dynamical cores, e.g. NCAR’s Model for Prediction Across Scales (MPAS),

- are formulated in z (constant volume) coordinates
- are non-hydrostatic
- include all condensates in pressure/density (a.k.a. condensate loading)
- use a discrete prognostic state different from physics package prognostic state

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How to couple dynamical core and physics package ensuring thermodynamic/energetic consistency?

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A. Issues from 1st principles

Continuous energy equations

Constant volume and constant pressure models/components conserve different energies.

In the absence of source and sinks constant volume and pressure models conserve

$$
\begin{aligned}
\frac{\partial}{\partial t}\iiint\left[K+c_v^{(d)}T+\Phi\right]\rho^{(d)}dA\,dz &= 0,\ z_t\ \text{constant}, \quad (35)\\
\frac{\partial}{\partial t}\iiint\left[K+c_v^{(d)}T+\Phi\right]\rho^{(d)}dA\,dz + \underbrace{\frac{1}{g}\frac{\partial}{\partial t}\iint p_t\Phi_t dA}_{\text{work done by } p \text{ at top}} &= 0,\ p_t\ \text{constant} \quad (36)
\end{aligned}
$$

(dry atmosphere)

Note: only difference between hydrostatic and non-hydrostatic energy is K (2D or 3D)!

B. Issues from 1st principles

Thermodynamic active water species discrepancy

Dynamical cores used for high resolution incl. condensate loading, however, most physics packages (I know of) do not:

$$\frac{\partial}{\partial t}\iiint \rho^{(d)} E_{feom}\, dA\, dz = \frac{\partial}{\partial t}\iiint \rho^{(d)} \left[\sum_{\ell \in \mathcal{L}_{all}} m^{(\ell)} \left(K + \Phi_s + c_p^{(d)} T \right) \right] dA\, dz$$

$$\mathcal{L}_{all} \equiv \{d, wv, cl, ci, rn, sw, gr\}$$

Dynamical core with condensate loading!

$$\sum_{\ell \in \{'d','wv'\}}$$

Physics package

B. Issues from 1st principles

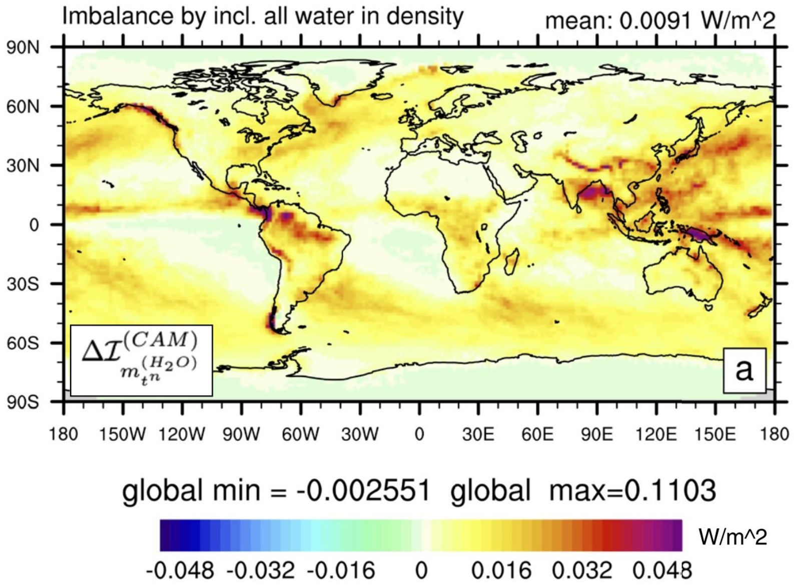
Thermodynamic active water species discrepancy

One year average of total energy tendency due to non-precipitating condensates at 1 degree horizontal resolution

-> Effect small
(but will increase locally at higher resolution)

Lauritzen et al. (2022)

$$\Delta\mathcal{I}^{(CAM)}_{m_{tn}^{(H_2O)}} = \int \left[\rho^{(d)}\left(\sum_{\ell\in\mathcal{L}_{cond}} \overline{m}_{tn}^{(\ell)}\right)\right]\frac{\partial}{\partial t}\left(\overline{K}+\overline{\Phi}_s + c_p^{(d)}\overline{T}\right)dz$$

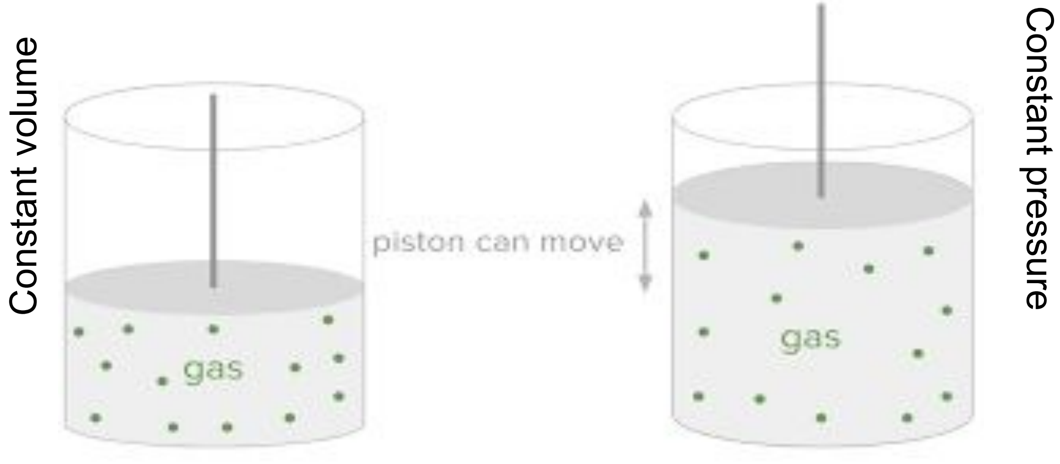


C. Issues from 1st principles

1st law of thermodynamics

Heating under constant volume and constant pressure lead to different temperature changes

Aside: carrying dT/dt as prognostic variable in physics packages is ambiguous (“bad” idea)!



Internal energy conservation

$$\frac{DU^{(d)}}{Dt} = \left.\frac{DQ}{Dt}\right|_{c_v^{(d)}T} - p^{(d)}\alpha^{(d)}\left(\nabla\cdot\vec{v} + \frac{\partial w}{\partial z}\right), \text{ (constant volume)}$$

Enthalpy conservation

$$\frac{Dh^{(d)}}{Dt} = \left.\frac{DQ}{Dt}\right|_{c_p^{(d)}T} + \alpha^{(d)}\omega^{(d)}, \text{ (constant pressure)}$$

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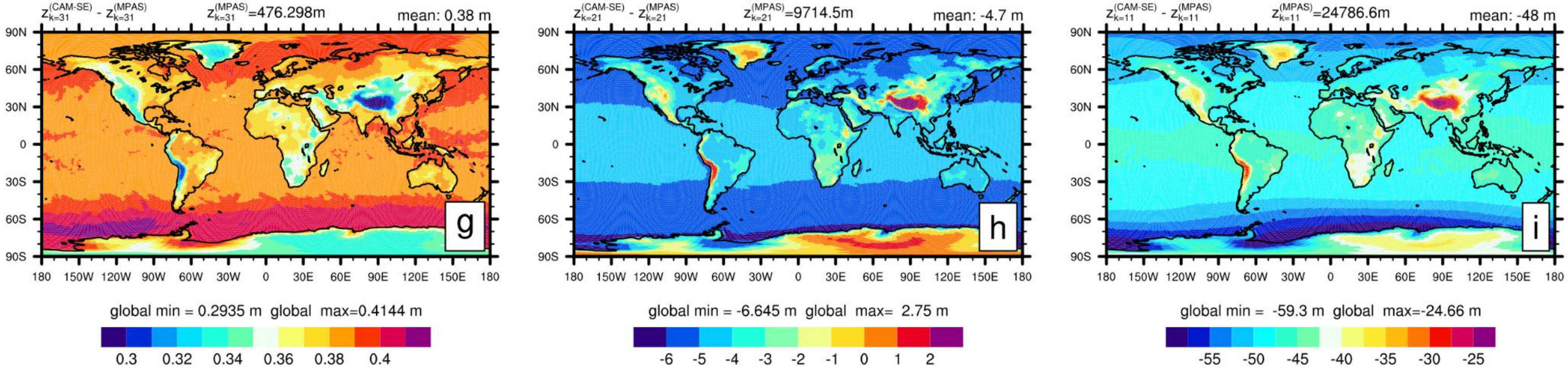
Discretization issue

Prognostic and diagnostics variables

Discrete representation of state in physics and dynamics may differ (both in terms of prognostic variables and staggering) which can lead to inconsistencies. Example:

$$\left(\theta_k^{(m)}, \vec{v}_k^{\perp}, \rho_k^{(d)}, z_{k+1/2}^{(MPAS)}, m_k^{(\ell)}\right) \qquad \left(T_k, \vec{v}_k, p_{k+1/2}, q_k^{(\ell)}, m_k^{(\ell)}\right)$$

Problem: z is fixed in MPAS whereas z is diagnosed (from hydrostatic balance) in CAM physics! If not careful in physics dynamics coupling -> z discrepancies. Example below:



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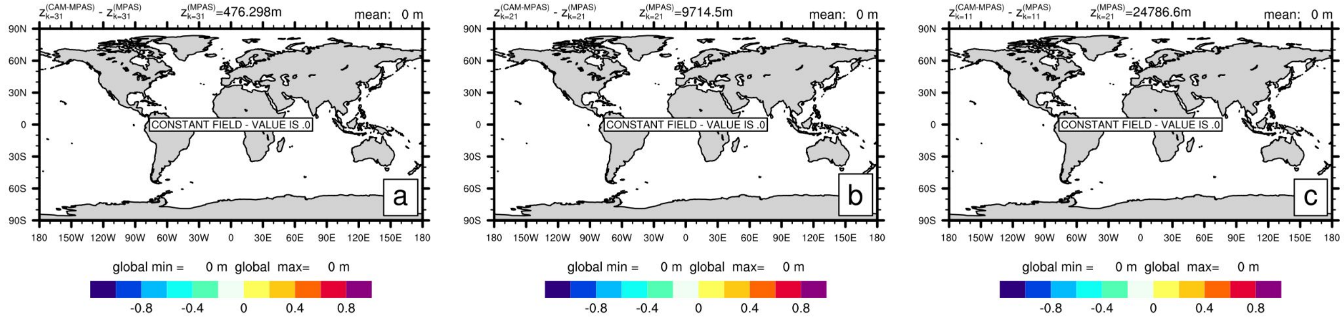
CAM-MPAS physics dynamics coupling

(addresses some consistency issues but not all)

See Lauritzen, Skamarock, … et al. (in prep) for details

- Preserving hydrostatic relations (heights diagnosed in physics consistent with MPAS dycore by cleverly choosing how the mid-level hydrostatic pressure is computed from MPAS state)



- Energy increments in physics (under constant pressure assumption) matching energy increment in hydrostatic MPAS (by scaling temperature increment and careful conversion from temperature tendency to modified potential temperature tendency used in MPAS)

- Making sure CAM physics energy fixer uses total energy formula consistent with hydrostatic MPAS

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Other (1st principle) issues that can be present in modeling systems that resolution will not “magically” fix …

D. Issues from 1st principles

Specific heat discrepancy

Lauritzen et al. (2022)

Some dynamical cores assume variable latent heats, i.e. they conserve the following total energy [e.g., FV3, NCAR Spectral-Elements (SE), …]

$$\frac{\partial}{\partial t}\iiint \rho^{(d)} E_{feom}\, dA\, dz = \frac{\partial}{\partial t}\iiint \rho^{(d)} \left[\sum_{\ell\in\mathcal{L}_{all}} m^{(\ell)}\left(K+\Phi_s+c_p^{(\ell)}T\right)\right] dA\, dz = 0.$$

(all enthalpy reference states, adiabatic dynamical core with inert water species)

whereas physics packages (I know of) use an energy formulation based on (constant latent heats):

$$\frac{\partial}{\partial t}\iiint \rho^{(d)} E_{feom}\, dA\, dz = \frac{\partial}{\partial t}\iiint \rho^{(d)} \left[\sum_{\ell\in\mathcal{L}_{all}} m^{(\ell)}\left(K+\Phi_s+c_p^{(d)}T\right)\right] dA\, dz$$

Example: this inconsistency leads to ~0.5W/m2 error in CAM-SE (Lauritzen and Williamson, 2019)

E. Issues from 1st principles

Important missing terms in total energy equation

Comprehensive total energy equation (using single temperature and single velocity assumptions):

Lauritzen et al. (2022)

$$\frac{\partial}{\partial t}\iiint \rho^{(d)}\left\{K+\Phi_s+c_p^{(d)}T+\sum_{\ell\in\mathcal{L}_{H_2O}} m^{(\ell)}\left[K+\Phi_s+c_p^{(\ell)}\left(T-T_{00}\right)+h_{00}^{(ice)}\right] +m^{(wv)}L_{s,00}+m^{(liq)}L_{f,00}\right\}dA\,dz$$

$$=\iint\left\{\sum_{\ell\in\mathcal{L}_{H_2O}} \underline{F_{net}^{(\ell)}}\left[\tilde{K}_s+\Phi_s+\underline{c_p^{(\ell)}\left(\tilde{T}_s-T_{00}\right)}+h_{00}^{(ice)}\right] +F_{net}^{(wv)}L_{s,00}+F_{net}^{(liq)}L_{f,00}+F_{net}^{(turb,rad)}\right\}dA.$$

$$\left(\text{ice reference enthalpy}, \tilde{T}_s\equiv T_{atm,s}=T_{surf,s}\right)$$

All physics packages (I know of) ignore the surface enthalpy flux terms (this term is locally large!)

Modern ocean models (e.g. MOM6, MPAS-O) do have explicit enthalpy flux terms …

E. Issues from 1st principles

Important missing term in total energy equation

Lauritzen et al. (2022)

Modified CAM total energy equation incl. missing flux terms

$$\frac{\partial}{\partial t}\int \overline{\rho}^{(d)}\left\{\left(1+\overline{m}^{(H_2O)}\right)\left[\overline{K}+\overline{\Phi}_s+c_p^{(d)}\left(\overline{T}-T_{00}\right)\right]+\overline{m}^{(wv)}L_{s,00}+\overline{m}^{(liq)}L_{f,00}\right\}dz$$

$$-\Delta\widehat{\mathcal{I}}_{\partial m^{(H_2O)}/\partial t}-\Delta\mathcal{I}_{m_{tn}^{(H_2O)}}=\overline{F}^{(H_2O)}_{net}\left[c_p^{(d)}\left(\widetilde{\overline{T}}_s-T_{00}\right)+\widetilde{\overline{K}}_s+\overline{\Phi}_s\right]+\overline{F}^{(wv)}_{net}L_{s,00}+\overline{F}^{(liq)}_{net}L_{f,00}+\overline{F}^{(turb,rad)}_{net}$$

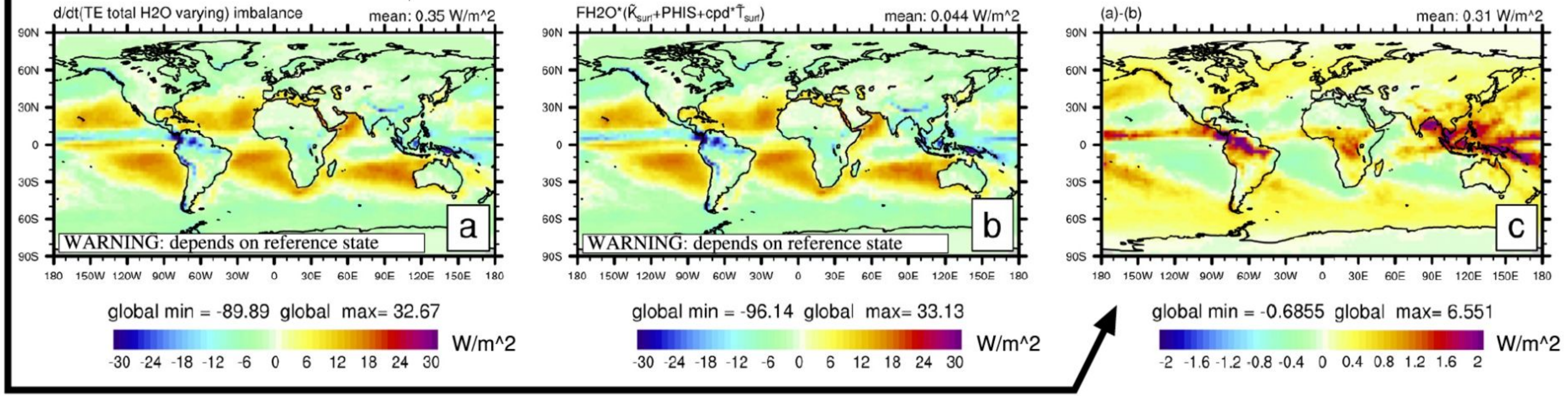
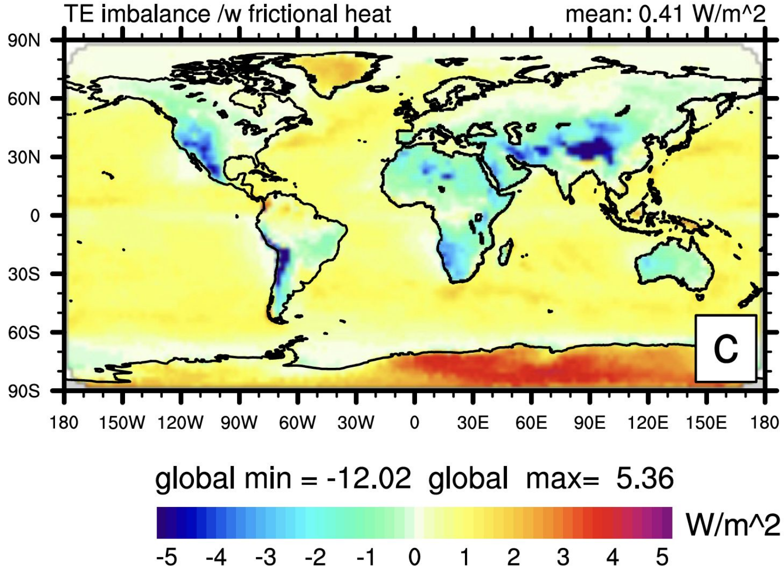


Figure 6. Modified (consistent) CAM total energy equation terms in W/m^2: (a) Imbalance introduced by “dry-mass adjustment” using all forms of water in the kinetic, geopotential and enthalpy terms, (b) missing flux terms, and (c) is the difference between (a and b). Note that the imbalance is locally much reduced when using the modified total energy equation. Also, the imbalance does not depend on the reference state (as should always be the case).

F. Issues from 1st principles

Thermodynamic inconsistency within physics

CAM physics conserves enthalpy (CAM's thermodynamic potential) which under constant pressure assumption leads to total energy conservation (in pressure coordinates). Parameterizations may conserve another thermodynamic variable (such as moist potential temperature; e.g. CLUBB = Cloud Layers Unified By Binormals does that) which is not consistent with the CAM physics total energy equation. This leads to discrepancies:



Lauritzen et al. (2022)

(G. Issues from 1st principles)

Dynamical cores do not inherently conserve total energy

Dynamical cores dissipate total energy (diffusion operators etc.). At 1 degree resolution modern dynamical cores dissipate ~0.3 - 1 W/m2. Luckily this error reduces at higher resolution (but, in my experience, only if resolution is increased in BOTH horizontal and vertical!)

Lauritzen et al. (2022)

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2.4 Heights derived from CAM physics state (temperature and pressure) consistent with MPAS height

The layer thickness Δz_k in CAM physics is diagnosed from the hydrostatic equation (13) by integrating it over layer k

Fixed in MPAS

$$\Delta z_k = \int_{z_{k+1/2}}^{z_{k-1/2}} dz, \quad (18)$$

$$\Delta p_k^{(h)} = g\Delta z_k \rho_k = g \Delta z_k \rho_k^{(d)} \sum_{\ell \in \mathcal{L}} m_k^{(\ell)}$$

$$= \int_{p^{(h)}_{k+1/2}}^{p^{(h)}_{k-1/2}} \frac{1}{\rho_k g} dp, \quad (19)$$

$$= \int_{p^{(h)}_{k+1/2}}^{p^{(h)}_{k-1/2}} \frac{R^{(d)} T_k^{(v)}}{g\,p} dp \quad (20)$$

$$= \frac{1}{p_k^{(h)}} \frac{R^{(d)} T_k^{(v)}}{g} \Delta p_k^{(h)}$$

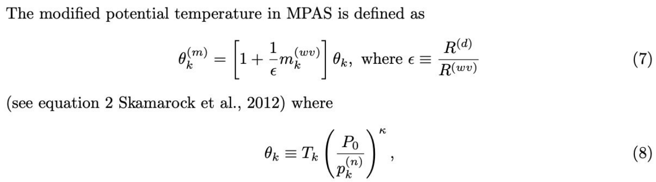
If we use non-hydrostatic pressure does NOT guarantee consistency:

$$p_k^{(n)} = \left[\rho_k^{(d)} R^{(d)} \theta_k^{(m)} / P_0\right]^{c_p^{(d)}/c_v^{(d)}} P_0.$$

Solution:

$$p_k^{(MPAS)} = -\frac{\Delta p_k^{(MPAS)}}{\Delta z_k^{(MPAS)}} \frac{R^{(d)} T_k^{(v)}}{g}$$

T diagnosed from modified potential T and non-hydrostatic mid-level p:



The modified potential temperature in MPAS is defined as

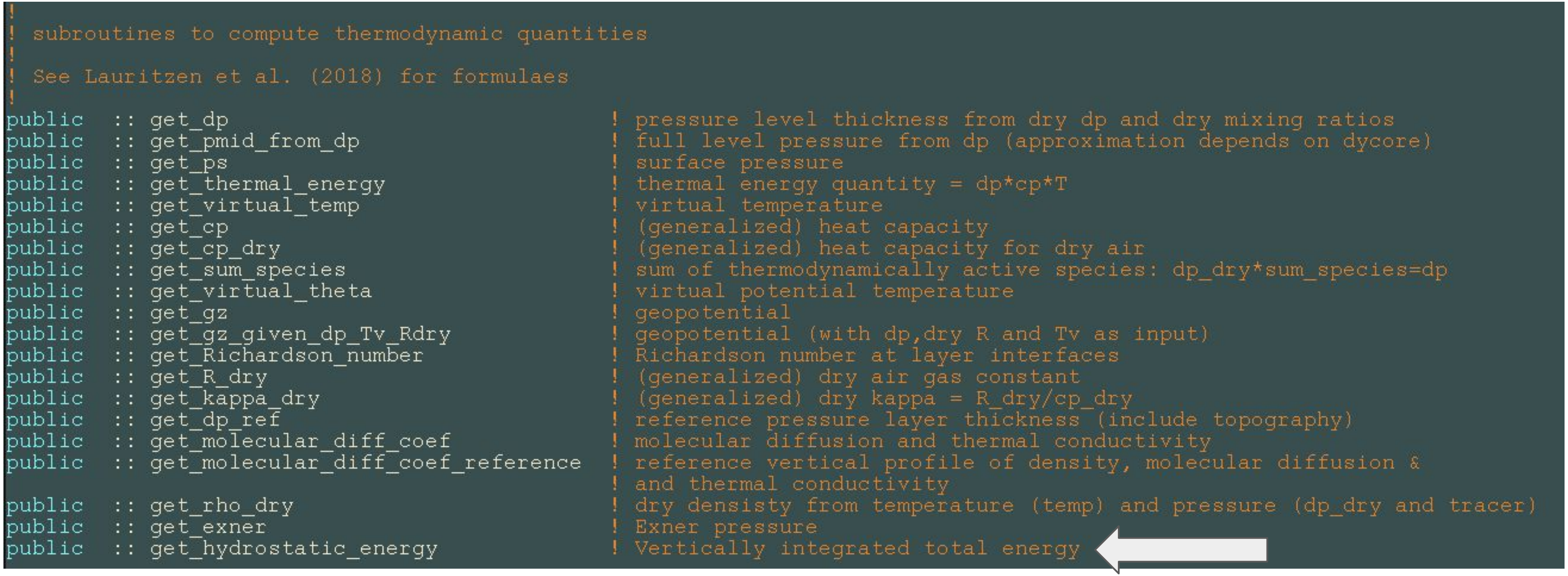
$$\theta_k^{(m)} = \left[1 + \frac{1}{\epsilon} m_k^{(wv)}\right] \theta_k, \text{ where } \epsilon \equiv \frac{R^{(d)}}{R^{(wv)}} \quad (7)$$

(see equation 2 Skamarock et al., 2012) where

$$\theta_k \equiv T_k \left(\frac{P_0}{p_k^{(n)}}\right)^{\kappa}, \quad (8)$$

Some infrastructures to start tackling these issues

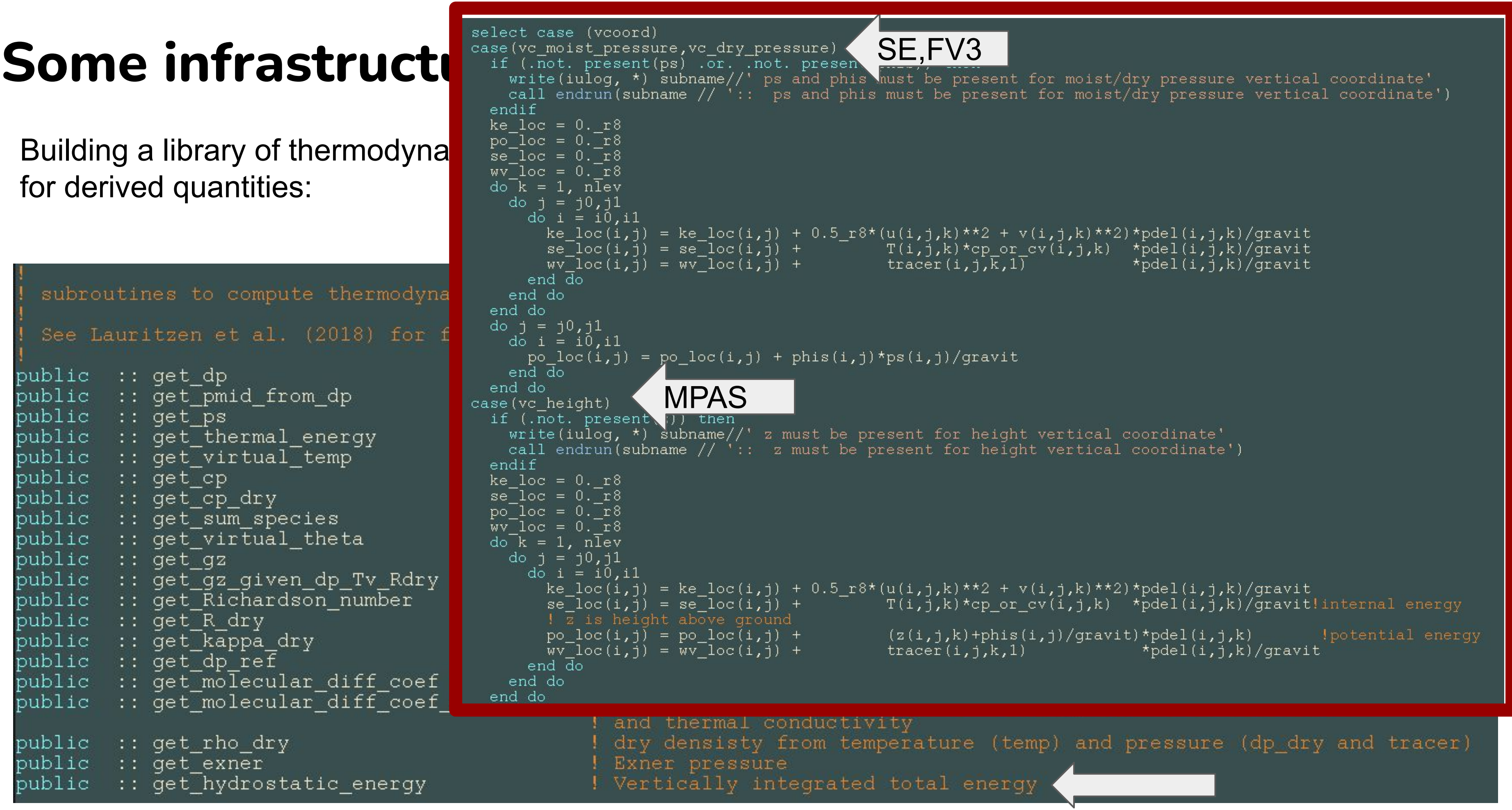
Building a library of thermodynamic functions and make sure that physics and dynamics call this library for derived quantities:



```
!
! subroutines to compute thermodynamic quantities
!
! See Lauritzen et al. (2018) for formulaes
!
public  :: get_dp                             ! pressure level thickness from dry dp and dry mixing ratios
public  :: get_pmid_from_dp                   ! full level pressure from dp (approximation depends on dycore)
public  :: get_ps                             ! surface pressure
public  :: get_thermal_energy                 ! thermal energy quantity = dp*cp*T
public  :: get_virtual_temp                   ! virtual temperature
public  :: get_cp                             ! (generalized) heat capacity
public  :: get_cp_dry                         ! (generalized) heat capacity for dry air
public  :: get_sum_species                    ! sum of thermodynamically active species: dp_dry*sum_species=dp
public  :: get_virtual_theta                  ! virtual potential temperature
public  :: get_gz                             ! geopotential
public  :: get_gz_given_dp_Tv_Rdry            ! geopotential (with dp,dry R and Tv as input)
public  :: get_Richardson_number              ! Richardson number at layer interfaces
public  :: get_R_dry                          ! (generalized) dry air gas constant
public  :: get_kappa_dry                      ! (generalized) dry kappa = R_dry/cp_dry
public  :: get_dp_ref                         ! reference pressure layer thickness (include topography)
public  :: get_molecular_diff_coef            ! molecular diffusion and thermal conductivity
public  :: get_molecular_diff_coef_reference  ! reference vertical profile of density, molecular diffusion &
                                              ! and thermal conductivity
public  :: get_rho_dry                        ! dry densisty from temperature (temp) and pressure (dp_dry and tracer)
public  :: get_exner                          ! Exner pressure
public  :: get_hydrostatic_energy             ! Vertically integrated total energy
```

Some infrastructu

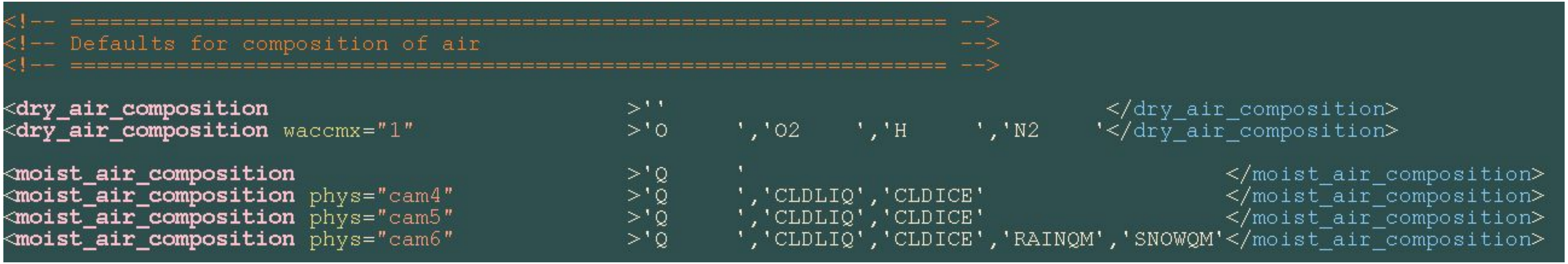
Building a library of thermodyna
for derived quantities:



```
!
! subroutines to compute thermodyna
!
! See Lauritzen et al. (2018) for f
!
public  :: get_dp
public  :: get_pmid_from_dp
public  :: get_ps
public  :: get_thermal_energy
public  :: get_virtual_temp
public  :: get_cp
public  :: get_cp_dry
public  :: get_sum_species
public  :: get_virtual_theta
public  :: get_gz
public  :: get_gz_given_dp_Tv_Rdry
public  :: get_Richardson_number
public  :: get_R_dry
public  :: get_kappa_dry
public  :: get_dp_ref
public  :: get_molecular_diff_coef
public  :: get_molecular_diff_coef_
                                              ! and thermal conductivity
public  :: get_rho_dry                        ! dry densisty from temperature (temp) and pressure (dp_dry and tracer)
public  :: get_exner                          ! Exner pressure
public  :: get_hydrostatic_energy             ! Vertically integrated total energy
```

```
select case (vcoord)
case(vc_moist_pressure,vc_dry_pressure)
  if (.not. present(ps) .or. .not. presen
    write(iulog, *) subname//' ps and phis must be present for moist/dry pressure vertical coordinate'
    call endrun(subname // '::  ps and phis must be present for moist/dry pressure vertical coordinate')
  endif
  ke_loc = 0._r8
  po_loc = 0._r8
  se_loc = 0._r8
  wv_loc = 0._r8
  do k = 1, nlev
    do j = j0,j1
      do i = i0,i1
        ke_loc(i,j) = ke_loc(i,j) + 0.5_r8*(u(i,j,k)**2 + v(i,j,k)**2)*pdel(i,j,k)/gravit
        se_loc(i,j) = se_loc(i,j) +         T(i,j,k)*cp_or_cv(i,j,k)  *pdel(i,j,k)/gravit
        wv_loc(i,j) = wv_loc(i,j) +         tracer(i,j,k,1)           *pdel(i,j,k)/gravit
      end do
    end do
  end do
  do j = j0,j1
    do i = i0,i1
      po_loc(i,j) = po_loc(i,j) + phis(i,j)*ps(i,j)/gravit
    end do
  end do
case(vc_height)
  if (.not. present( )) then
    write(iulog, *) subname//' z must be present for height vertical coordinate'
    call endrun(subname // '::  z must be present for height vertical coordinate')
  endif
  ke_loc = 0._r8
  se_loc = 0._r8
  po_loc = 0._r8
  wv_loc = 0._r8
  do k = 1, nlev
    do j = j0,j1
      do i = i0,i1
        ke_loc(i,j) = ke_loc(i,j) + 0.5_r8*(u(i,j,k)**2 + v(i,j,k)**2)*pdel(i,j,k)/gravit
        se_loc(i,j) = se_loc(i,j) +         T(i,j,k)*cp_or_cv(i,j,k)  *pdel(i,j,k)/gravit!internal energy
        ! z is height above ground
        po_loc(i,j) = po_loc(i,j) +         (z(i,j,k)+phis(i,j)/gravit)*pdel(i,j,k)       !potential energy
        wv_loc(i,j) = wv_loc(i,j) +         tracer(i,j,k,1)            *pdel(i,j,k)/gravit
      end do
    end do
  end do
```

A generalized implementation of thermodynamics for species dependent air (dry air composition and condensates) using namelist



```
<!-- ================================================================= -->
<!-- Defaults for composition of air                                   -->
<!-- ================================================================= -->

<dry_air_composition                          >''                                 </dry_air_composition>
<dry_air_composition waccmx="1"               >'O     ','O2    ','H     ','N2    '</dry_air_composition>

<moist_air_composition                        >'Q     '                                    </moist_air_composition>
<moist_air_composition phys="cam4"            >'Q     ','CLDLIQ','CLDICE'                  </moist_air_composition>
<moist_air_composition phys="cam5"            >'Q     ','CLDLIQ','CLDICE'                  </moist_air_composition>
<moist_air_composition phys="cam6"            >'Q     ','CLDLIQ','CLDICE','RAINQM','SNOWQM'</moist_air_composition>
```

Namelist specification of the composition of air, i.e. one can “easily” change composition of air and thermodynamically active water species (note: also applicable to other planets)

SE dynamical core and CAM-WACCM physics call the same module to get molecular viscosity and thermal conductivity coefficients, generalized cp and R, pressure (incl. weight of condensates if applicable), etc.

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