RRTMG-P: An Updated and Standardized Radiative Transfer Package for Earth System Applications on High Performance Computing Systems

Robert Pincus
University of Colorado
Brian Eaton
NCAR/CGD
John Dennis, Youngsung Kim
NCAR/CISL
John Michalakes
(michalak@ucar.edu)
UCAR/CPAESS and NRL

18th WRF Users Workshop
13 June 2017

RRTMG*P* Project

ONR/NOPP-funded: “RRTMGP: A High Performance Broadband Radiation Code for the Next Decade” *

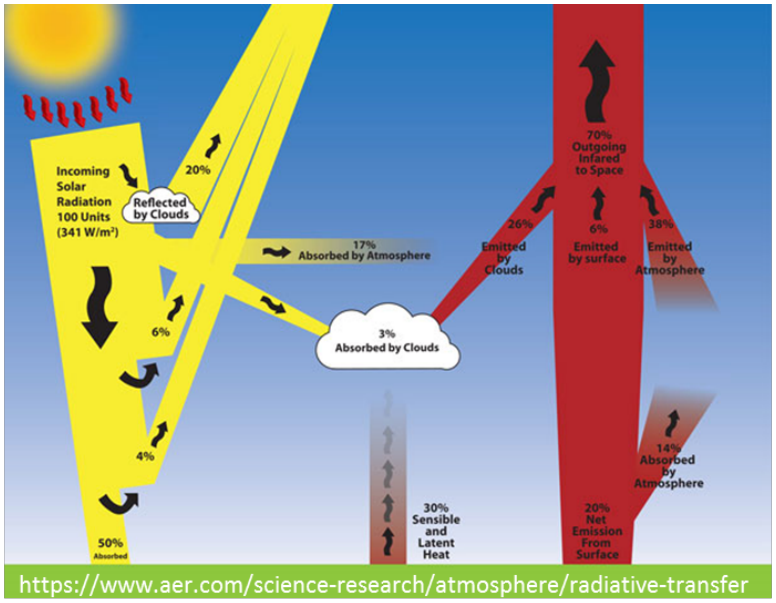
- Update science and software of AER’s widely used but 20-year old Rapid Radiative Transfer Model (background on next slide)
- 2013-2016, $625K between AER, U. Colorado, and NCAR
  - Continuing now under 2-year follow-up grant
  - Also some NASA support
- Implementation in Community Atmosphere Model of CESM is nearing completion
- Active interest: ICON (DWD), GFS (NCEP), NEPTUNE (NRL)

* Mlawer, Berthiaume, Pincus, Eaton, Liu, and Iacono https://www.earthsystemcog.org/projects/espc-aoli/2013_meeting

Background

RRTMGP* builds upon and updates science and software of the 20 year old Rapid Radiative Transfer Model (RRTMG)**

- K-distribution treatment of absorption and emission by gases as a function of temperature, pressure, etc, coupled to two-stream methods for computing radiation transport
- Expensive but highly efficient compared to the reference Line-by-Line RTM
- RRTMG is widely adopted: NCEP, NASA, ECMWF, CESM, and WRF but each group has a different version of the software and these are diverging
- Experimental versions of RRTMG ported/ optimized for next-generation processors (MIC, GPU) ***



* Mlawer, Berthiaume, Pincus, Eaton, Liu, and Iacono https://www.earthsystemcog.org/projects/espc-aoli/2013_meeting

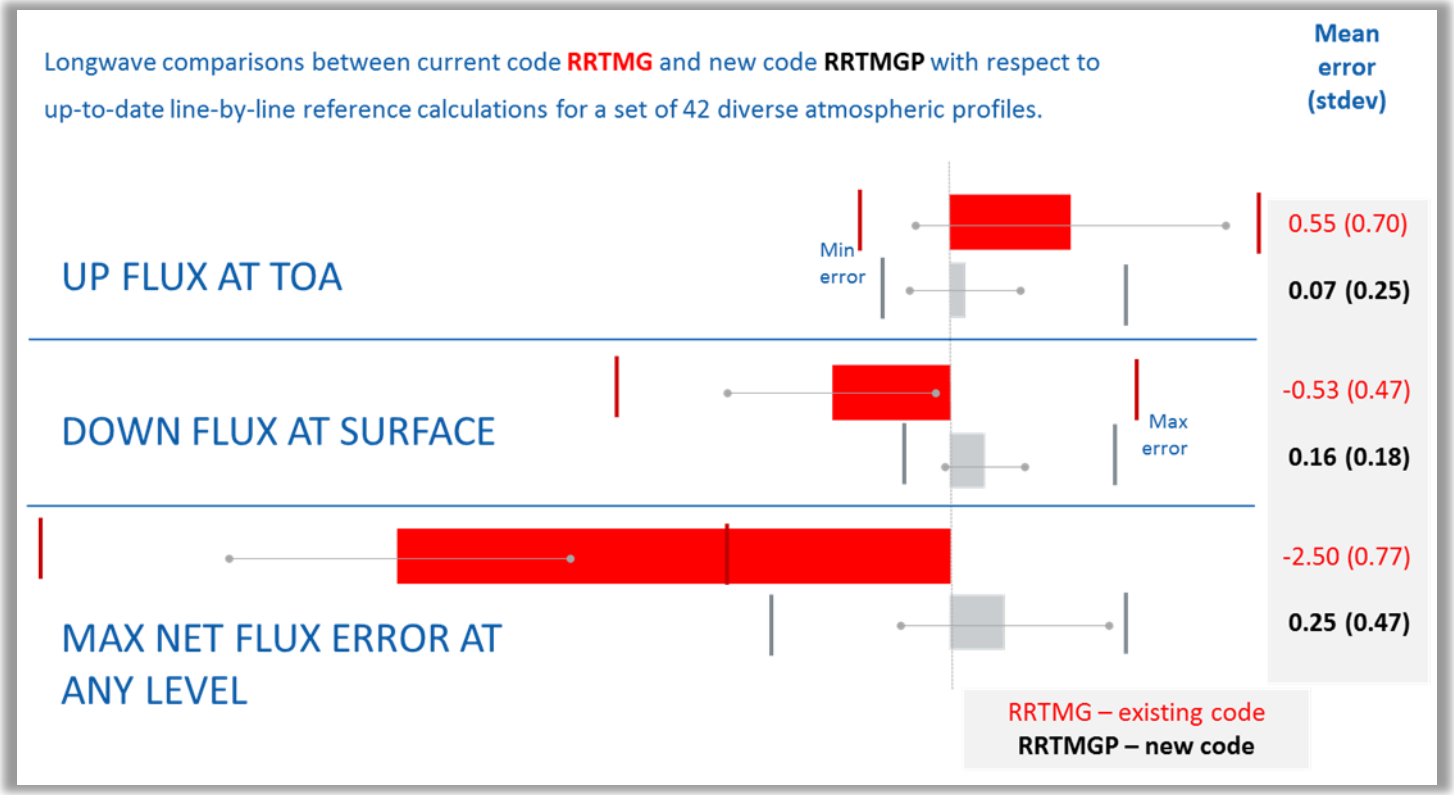
** Mlawer, Taubman, Brown, Iacono, and Clough. *Journal of Geophysical Research: Atmospheres.* vol. 102, no. D14, 1997.

*** Michalakes, , Iacono, Jessup. Parallel Processing Letters, 26 No. 4. World Scientific. Dec. 2016. http://dx.doi.org/10.1142/S0129626416500195

RRTMG*P* Science Improvements

RRTMGP is based on latest spectroscopic knowledge

- Aer_v3.5 * based on HITRAN 2012 ** (vs. HITRAN 2002 for RRTMG)
- Newly validated against Line-by-Line RTM



* AER Line Parameter Database: http://rtweb.aer.com/line_param_frame.html

** The HITRAN Database: https://www.cfa.harvard.edu/hitran/facts.html

RRTMG*P* Software Improvements

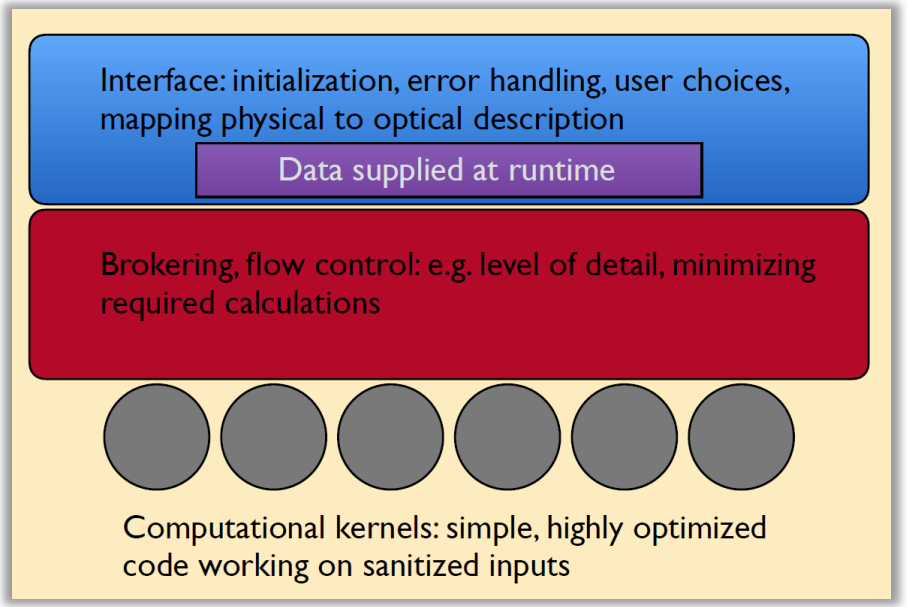
Seeks to balance efficiency and flexibility

- Increased efficiency:
  - RRTMGP computational kernels structured to take advantage thread and fine-grain parallelism of new HPC architectures
- Improve flexibility and modularity of the code:
  - Entirely new code using Fortran 2003 Objected Oriented features
  - Models specify clouds, aerosols, gas concentrations by calling “init” methods defined in RRTMGP classes
  - RRTMGP may be built and used as a library that need not be changed for different models and applications
- Allows the currently numerous and divergent applications of the RRTMG to be updated to a single AER-supported community version RRTMGP software for HPC systems

RRTMG*P* Software Improvements

Flexibility: Object oriented brokering layer and interfaces written using Fortran 2003 classes to describe optical and physical properties of clouds, aerosols

- RRTMGP provides classes for
  - Optical properties that can be used directly (RRTMG provides)
  - Abstract and example classes for aerosols, clouds, random numbers (Model developer provides)
  - Output classes that can be extended as needed
  - Computational kernels
  - Example ... (next slide)



RRTMG*P* Software Improvements

Example model code that uses RRTMGP classes to initialize and then call RRTMGP shortwave radiation

```
type(ty_gas_optics) :: kdist_sw
type(ty_gas_conc) :: gas_concs
type(ty_fluxes) :: fsw, fswc
type(ty_optical_props_cld) :: cloud_sw   ! extended from RRTMGP class
ty_optical_props
...
!< Set gas volume mixing ratios
error = gas_concs%set_vmr('h2o', wv_vmr)
error = gas_concs%set_vmr('co2', 400.*1.e-6)

! Cloud optical properties
!
error = cloud_sw%init(ncol, nlay, kdist_sw%get_ngpt())
call compute_cloud_optics(cloud_fraction, cloud_lwp, &
                          cloud_sw%tau, cloud_sw%ssa, cloud_sw%g, ... )

! Call the RRTMGP shortwave routine
errmsg = rrtmgp_sw( &
  kdist_sw, gas_concs, pmid_rad, t_rad, pint_rad, &
  ... mu0,  sfc_alb_dir, sfc_alb_dif,  &
  ... cloud_sw, fsw, fswc, ... )
```

Blue: provided by or extended from RRTMGP

RRTMG*P* Software Improvements

Example model code that uses RRTMGP classes to initialize and then call RRTMGP shortwave radiation

```
type(ty_g
type(ty_g
type(ty_f
type(ty_c
ty_optica
...
!< Set gas vo
error = g
error = g

! Cloud optic
!
error = c
call comp
```

```
type, public :: ty_gas_optics
  real, dimension(:,:,:), allocable :: tau ! optical depth
  real, dimension(:,:,:), allocable :: ssa ! single-scattering albedo
  real, dimension(:,:,:), allocable :: g   ! asymmetry  parameter
    ...
contains
  procedure, public :: init
  procedure, public :: get_ncol, get_nlay, get_ngpt
    ...
 end type ty_gas_optics_specification
```

```
cloud_sw%tau, cloud_sw%ssa, cloud_sw%g, ... )

! Call the RRTMGP shortwave routine
errmsg = rrtmgp_sw( &
  kdist_sw, gas_concs, pmid_rad, t_rad, pint_rad, &
  ... mu0,  sfc_alb_dir, sfc_alb_dif,  &
  ... cloud_sw, fsw, fswc, ... )
```

Blue: provided by or extended from RRTMGP

RRTMG*P* Efficiency Improvements

Efficiency: redesigned computational kernels (solvers and other core routines) for efficiency on next generation architectures

- Parallelism over adjacent columns as innermost dimension that allows efficient use of Intel's AVX vector instructions and SIMT threads on NVIDIA's GPGPU architecture
- Thread safe software modules, can be called within threaded regions of host models
- May involve trading off maximum performance for software flexibility, but goal is to at least match the performance of current RRTMG codes
- Single source code designed for efficiency on multiple platforms

Computational Performance (Longwave)

- Current kernel cost:
  - Baseline
    - `RRTMG:  5.2 milliseconds`
    - `RRTMGP:  24.8 milliseconds (4.8x slower)`
- Observations
  - RRTMGP performs 4.4x more instructions
    - Two full executions, once for clearsky and once for cloudy (RRTMG combines these)
    - Twice as many g-points as RRTMG (this is being addressed)

Workload

Number of columns = 31

Number of layers = 16

Platform

Yellowstone of NCAR

Intel(R) Xeon(R) CPU E5-2670 0 @ 2.60GHz

RRTMG LW and RRTMGP LW are extracted as kernels from CESM's CAM using KGEN *

Performance is measured on a single core using the kernels

Extrae**/Folding is used for performance analysis

* Kim *et al.*, *Procedia Computer Science*, **80**, 2016 doi:10.1016/j.procs.2016.05.466

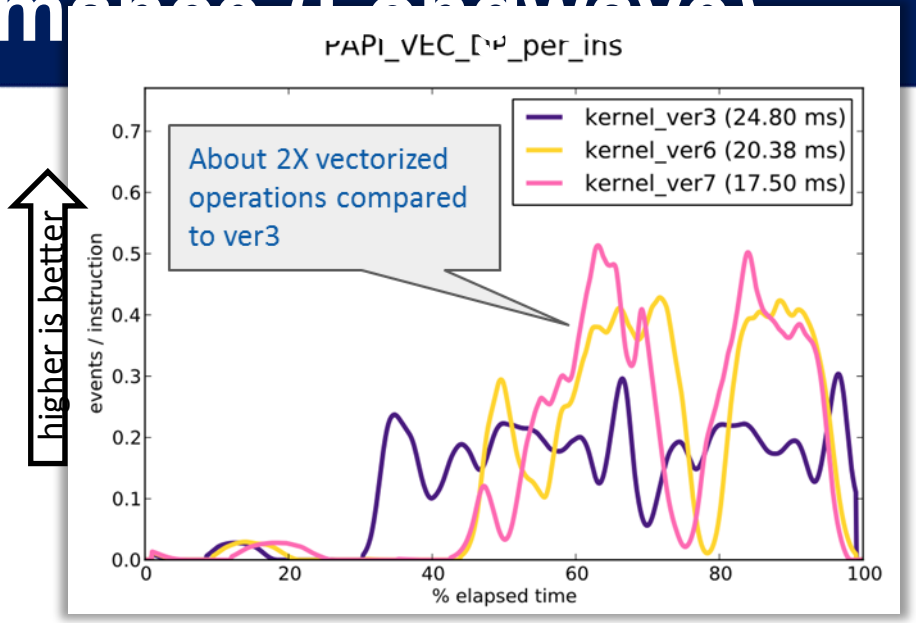
**Barcelona Supercomputing Center

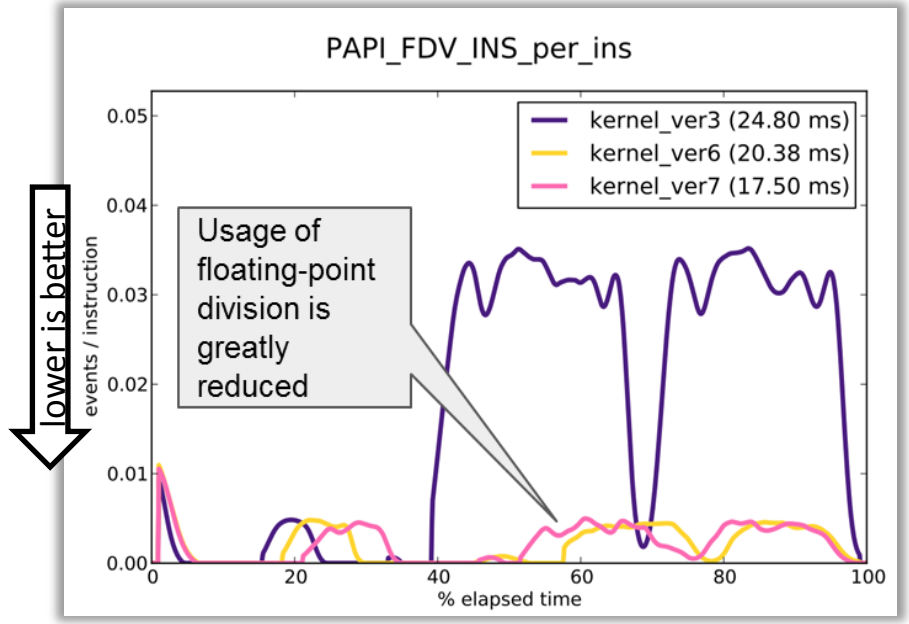
http://www.vi-hps.org/Tools/Extrae.html

Computational Performance (Longwave)

- Current kernel cost:
  - Baseline
    - `RRTMG:  5.2 milliseconds`
    - `RRTMGP:  24.8 milliseconds (4.8x slower)`
- Optimizations to date
  - Increased vector utilization in solver
  - Reduced number of floating point divisions in solver
  - Improve L2 cache reuse in gas-optics
    - **`RRTMGP:  17.5 milliseconds (3.4x slower)`**

More improvement needed, but on a per-instruction basis, the performance of RRTMGP is similar to RRTMG





RRTMG*P* Status and Future Work

- Readiness for community use
  - Coming soon

    Incorporating into real applications will begin once spectroscopic data has been finalized later this summer for longwave and in the fall for shortwave radiation
  - Continued performance improvement (Pincus with NCAR/CISL)
  - Prototype implementation in Community Atmosphere Model of CESM (NCAR/GSD) but won't be ready for CMIP6
  - NCEP and NRL also tracking development
  - RRTMGP should be available for initial testing in WRF later this year
- Todo: make conforming with NUOPC Physics Interface (potentially part of the Navy project).