A targeted machine learning approach to accelerate radiation computations

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Climate models are slow, and we should care

- Trend towards higher resolution in weather/climate models

- High-resolution simulations are highly energy intensive: on the state-of-the-art COSMO model run on efficient GPUs at 1 km resolution, 596 MWh per simulated year[1]

  → energy required to simulate 100 years could power 16000 UK homes for a year

- Trend towards more heterogenous and parallel hardware which legacy codes make poor use of (current NWP models realize a few % of peak performance[2])

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Atmospheric radiation: understood, but complex

- Radiative transfer is often one of the most expensive components in large-scale models (50% of runtime in ECHAM[3])

- This is despite using several tricks to simplify the well-understood but complex physics in modern radiation schemes

  - Treat radiation as 1D despite being 3D
  - To get around spectral complexity (millions of absorption lines), use the *correlated-k* method to reorder absorption coefficients in ascending order → *O*(2-3) pseudo-monochromatic spectral point (g-points)

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Machine learning to the rescue?

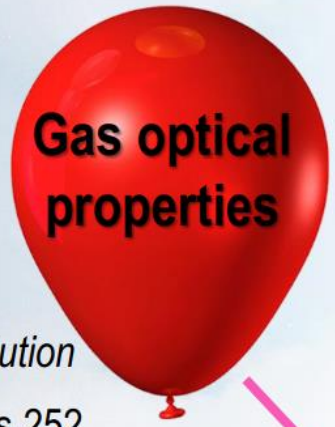
- Neural nets have been used to emulate entire radiation schemes (Krasnopolsky et al. (2010), Pal et al., (2019)..)

- Large speed-ups (10-100x) but at the cost of accuracy and generalization (20 W m^{-2} error in surface flux in Pal et al.)
  - Even small errors can accumulate

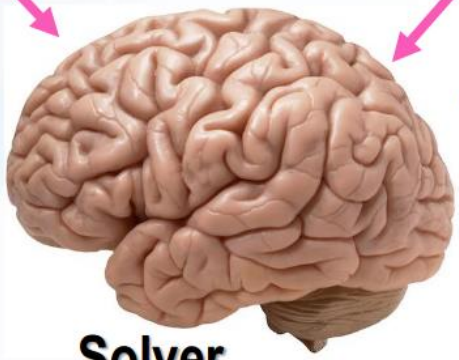
- Operational use would require high accuracy, stability and generalisation (to e.g. warmer climates)

- Alternative to the tall task of emulating the entire radiation code?

The four components of a radiation scheme



- *Determines spectral resolution*
- RRTM-G uses 252 spectral intervals



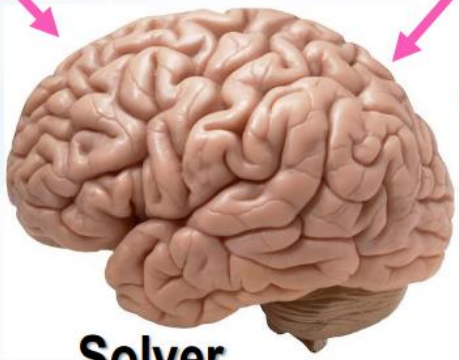
- *Determines how sophisticated interactions with clouds will be*

- Codes should be *modular*, allowing components to be changed independently

The four components of a radiation scheme

Interpolated from look-up-table

- *Determines spectral resolution*
- RRTM-G uses 252 spectral intervals



Physical equations for radiative transfer between layers

- *Determines how sophisticated interactions with clouds will be*

- Codes should be *modular*, allowing components to be changed independently

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Work in a nutshell

- Develop neural networks to replace the computation of optical properties in a new radiation scheme, RTE+RRTMGP
  - RRTMGP (RRTM for General circulation model applications—Parallell) is successor to RRTMG, used widely in GCM and NWP
  - RRTMGP computes optical properties of the atmosphere using (256+224=480) g-points
  - RTE (Radiative Transfer for Energetics) uses two-stream equations to compute radiative transfer
- Combine this with refactoring/optimizing other parts of the code

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Why NNs are (hopefully) more efficient

Original code maps atmospheric conditions to optical properties using LUT interpolation within lots of loops

- For each layer $j = 1...J$ in each column $k = 1...K$
  - For band $b = 1...B$
    - Compute the g-point vector $\overline{\tau, maj}_{b,j,k}$ by 3D linear interpolation in T, p and η.
    - For each minor gas
      - Compute τ_{min} by 2D linear interpolation in temperature and η
    - $\tau_{i,j,g} = \tau_{maj} + \tau_{min}$

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With NNs we can:

- Predict all g-points (224-256) and gas contributions (4-16) simultaneously
  $\mathbf{Y}_{ng} = f(\mathbf{X}_{ngas})$, where Y and X are vectors and *f* is the NN mapping
- (!) Since optical property computations are independent for model levels and columns, we can furthermore collapse nlev and ncol into one dimension *k* and do batch predictions for $\mathbf{Y}_{ng,k}$
- The core computations are then **matrix-matrix multiplications** which we can delegate to an optimized library (BLAS)

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Developing NNs to replace a physics scheme: lots of data needed!

- Obtain atmospheric profiles (T, p, q(H_2O), q(O_3), q(CO_2),..) from many sources
  - Reanalyses
  - climate projections
  - Idealized profiles
  - Sample present-day, preindustrial, future, LGM..
- Expand data synthetically: hypercube sampling of gas concentrations, tweak temps and humidities etc.

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- Expand data synthetically: hypercube sampling of gas concentrations, tweak temps and humidities etc.
- Use RRTMGP to compute outputs (absorption coefficients, emission)

  → 7 million training samples spanning **a large range** of atmospheric conditions

Accuracy

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After lots of experimenting, good results (R^2 >0.99) by using separate neural nets to predict molecular (=independent of layer thickness):

- LW (=longwave, terrestrial) absorption
- LW emission
- SW (=shortwave,solar) absorption
- SW scattering

Each NN outputs a vector of sizes 224 or 256, has 2 hidden layers and 18-64 neurons, and both inputs and outputs were scaled

e.g. log(p), $\sqrt{q(H_20)}$

+normalization

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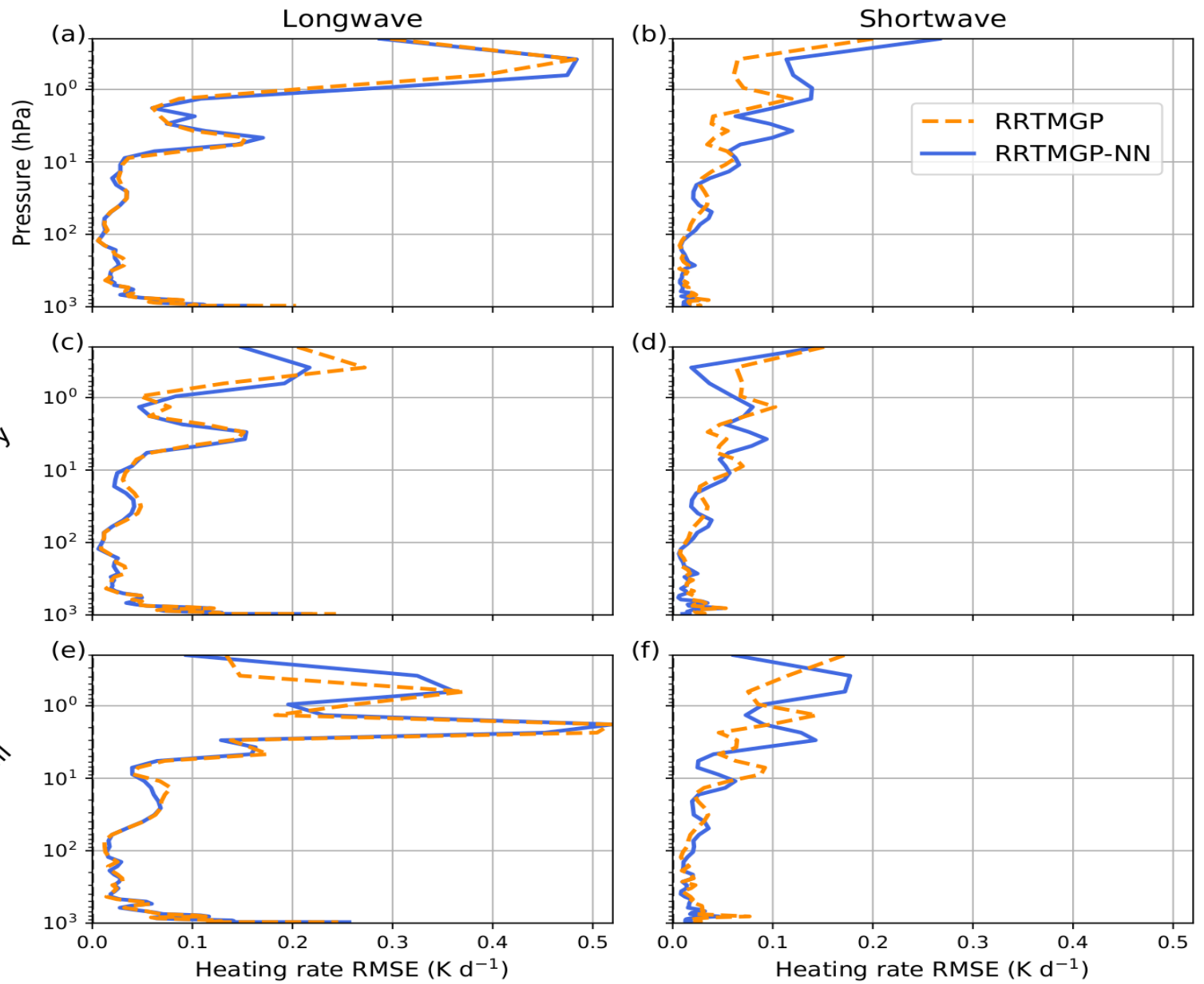

Accuracy (LW)

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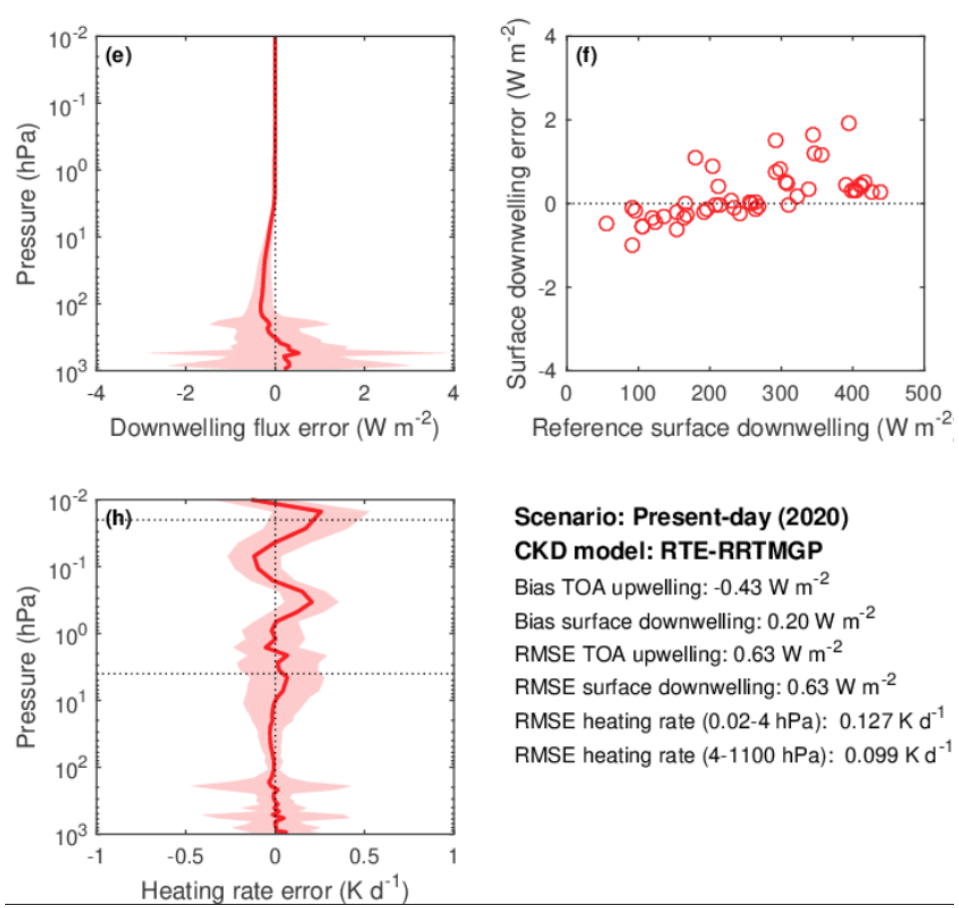
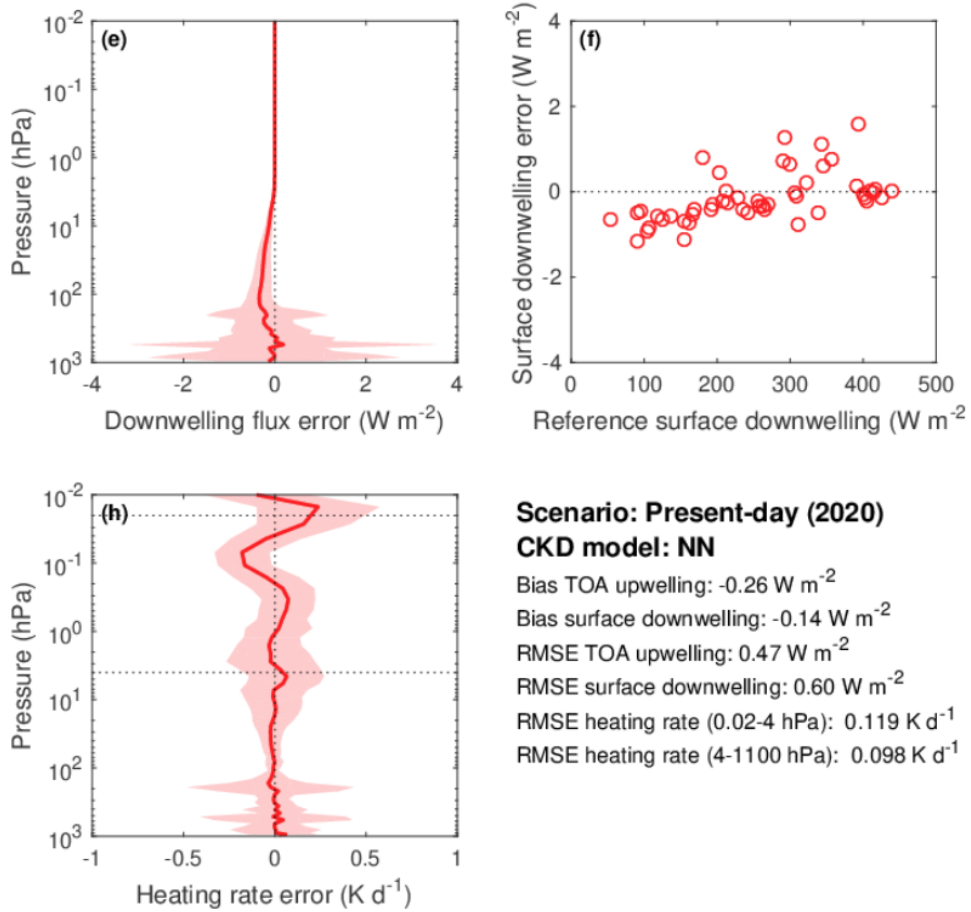
REFERENCE



Scenario: Present-day (2020)
CKD model: RTE-RRTMGP

Bias TOA upwelling: -0.43 W m^{-2}
Bias surface downwelling: 0.20 W m^{-2}
RMSE TOA upwelling: 0.63 W m^{-2}
RMSE surface downwelling: 0.63 W m^{-2}
RMSE heating rate (0.02-4 hPa): 0.127 K d^{-1}
RMSE heating rate (4-1100 hPa): 0.099 K d^{-1}

NEURAL NET



Scenario: Present-day (2020)
CKD model: NN

Bias TOA upwelling: -0.26 W m^{-2}
Bias surface downwelling: -0.14 W m^{-2}
RMSE TOA upwelling: 0.47 W m^{-2}
RMSE surface downwelling: 0.60 W m^{-2}
RMSE heating rate (0.02-4 hPa): 0.119 K d^{-1}
RMSE heating rate (4-1100 hPa): 0.098 K d^{-1}

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Implementation: neural networks in Fortran is simple and performance portable

- Neural nets were trained in Python, need to be used in Fortran

- I took an existing OO Fortran implementation of dense neural networks (neural-Fortran[4]), wrote new kernels using BLAS for batched inference

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Implementation: neural networks in Fortran is simple and performance portable

- GPUing the code is trivial

1) Call NVIDIAs cuBLAS instead of BLAS

2) OpenACC directives above loops

```
#ifdef USE_OPENACC
  use cublas
  use openacc
#define sgemm cublassgemm
#endif
```

```
! 1. Multiply inputs with weights of first layer

!$acc host_data use_device(wt, x, a)
call sgemm('N','N', neurons, nbatch, nx, 1.0, wt, neurons, x, nx, 0.0, a, neurons)
!$acc end host_data

! 2. Add biases and activation

!$acc parallel loop gang vector collapse(2) default(present)
do j = 1, nbatch
  do i = 1, neurons
    a(i, j) = a(i, j ) + b(i)
    call activation_softsign(a(i, j))
  end do
end do

! 3. Repeat steps 1-2 until final layer reached

do n = 3, nlayers-1
```

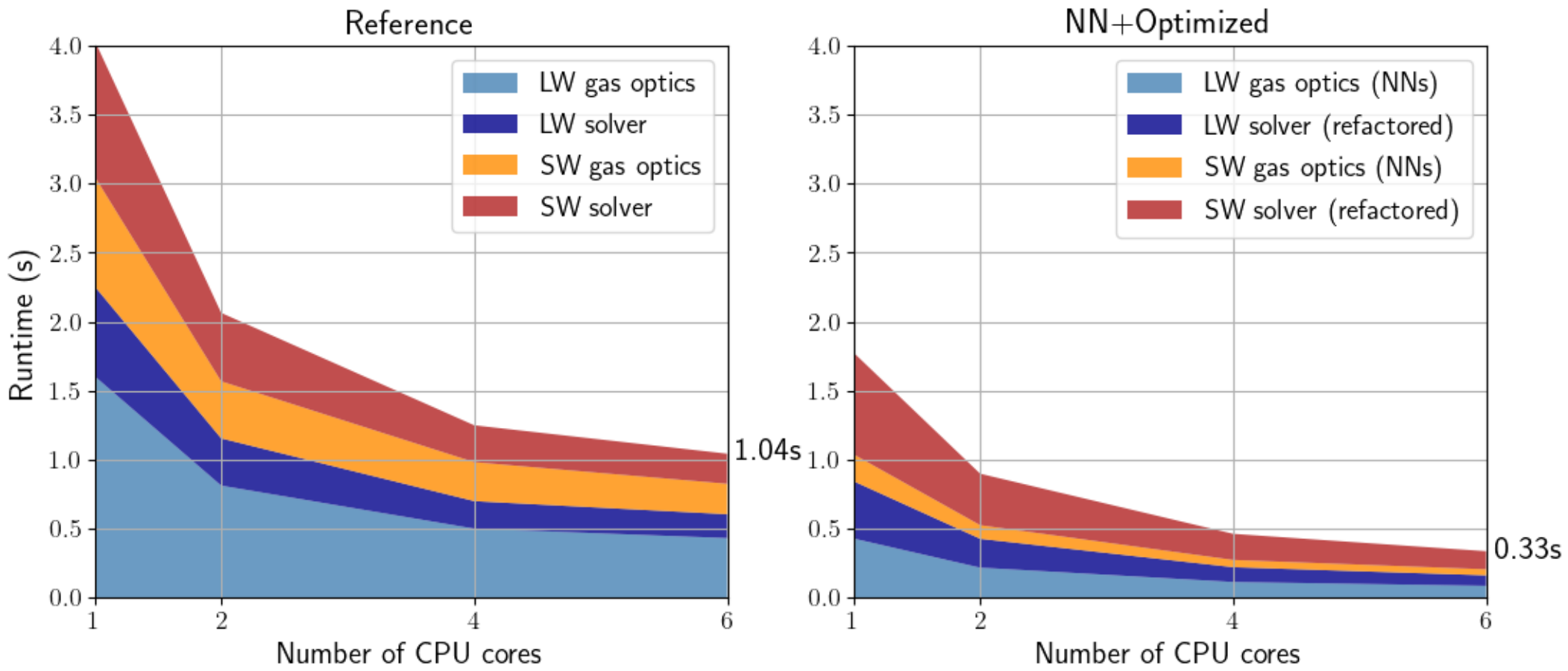
Code refactoring: switch around dimensions, pretty much

- The original RTE code uses columns as inner dimension, but RRTMGP has columns as outer dimension

  optical_depth(ng, nlev, ncol), radn_up(ncol, nlev, ng)

- In between expensive array transposes are needed. This motivated rewriting RTE to columns-last

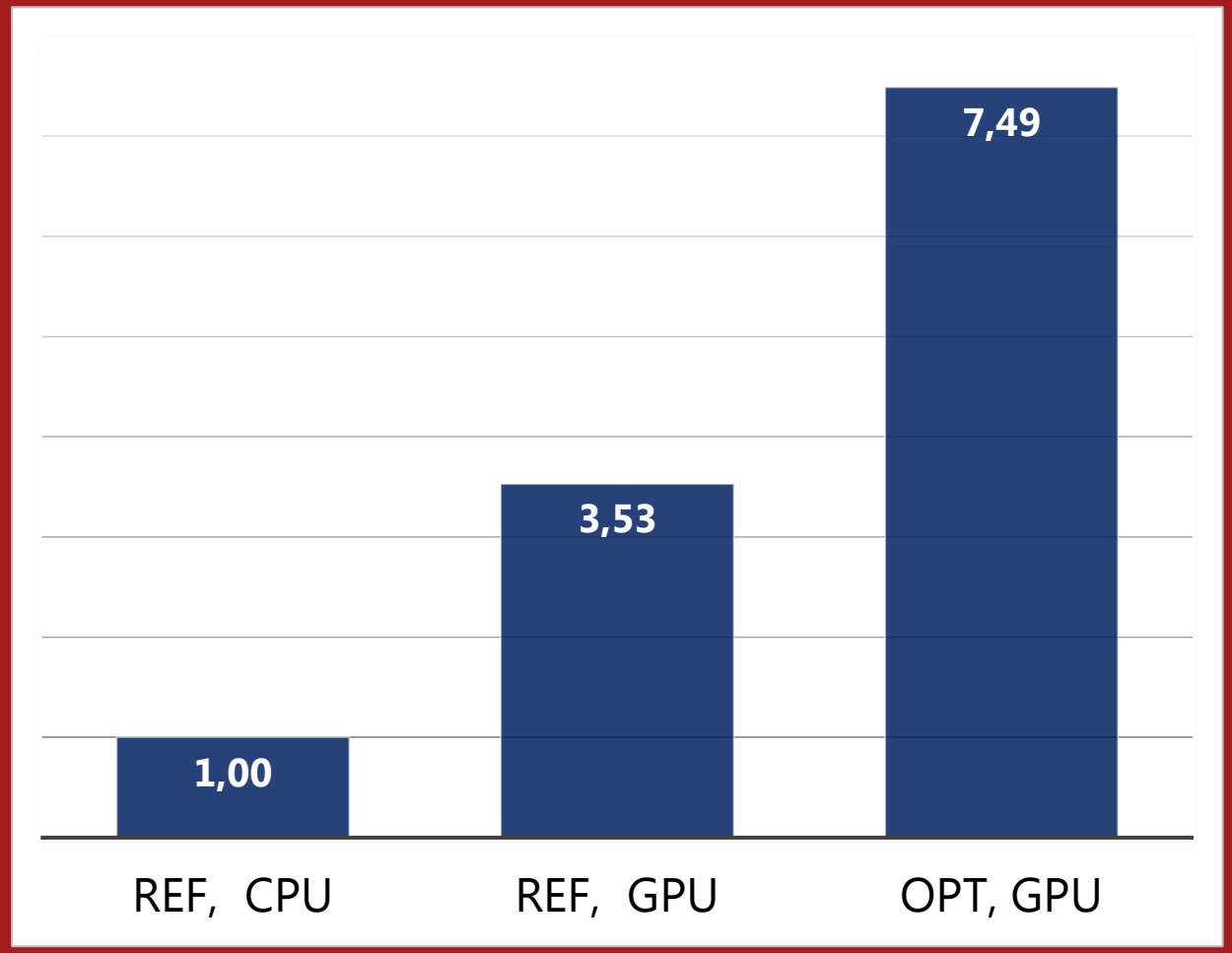
Time to solution, clear-sky computations for 6400 columns



CPU: AMD Ryzen 2600
Compiler: GCC 9.3, -O3
BLAS library: BLIS

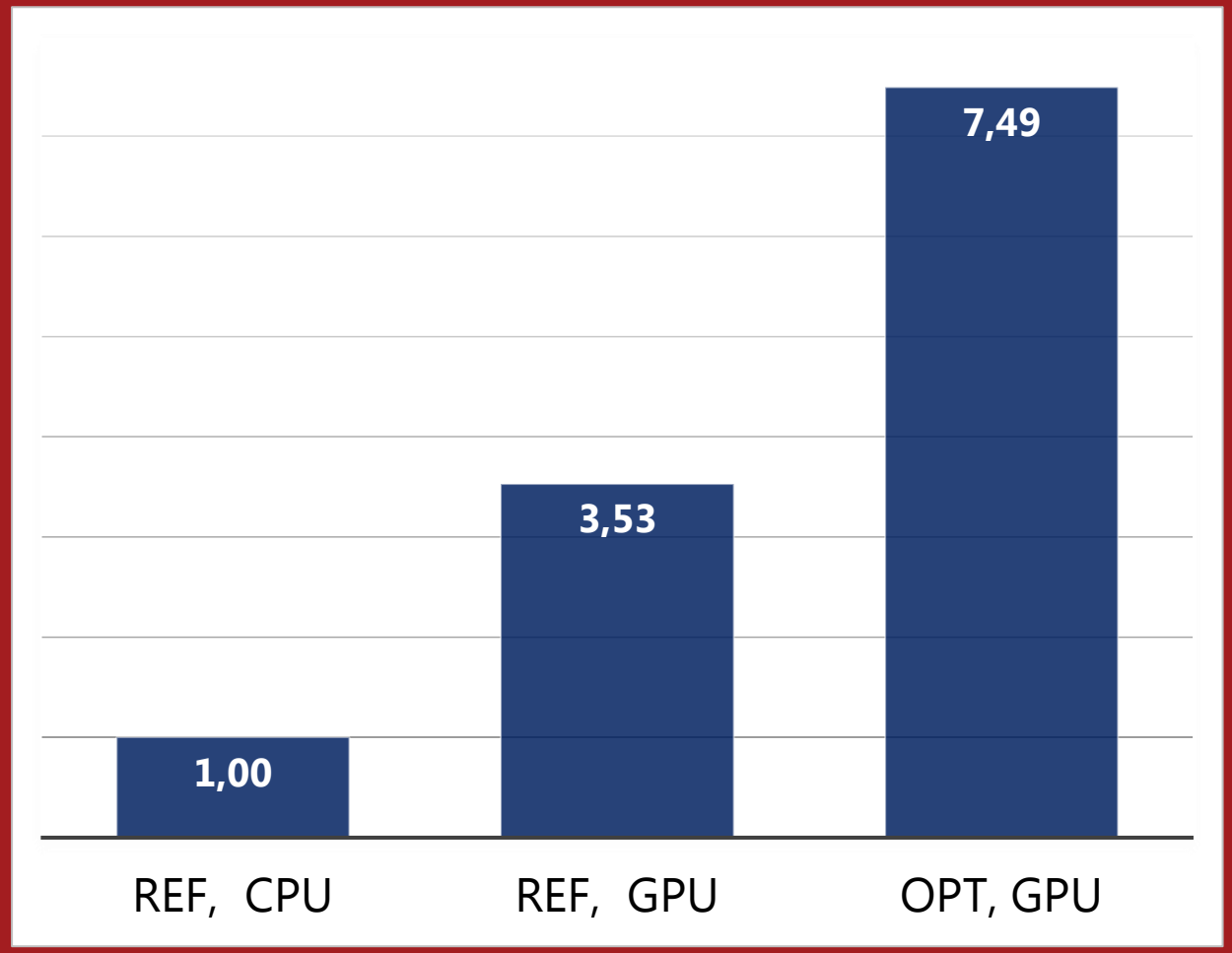
Only shortwave (SW) computations include scattering

Speed-up factor over REF (CPU)



CPU: Ryzen 2600, 6 cores
GPU: GTX 1070 (no tensor cores!)

Speed-up factor over REF (CPU)



The new gas optics has high computational efficiency due to BLAS
- 50 GFLOPS vs 5 GFLOPS for original kernel!

The ECMWF radiation scheme is even worse: 1-2 GFLOPS (but improvements are coming)

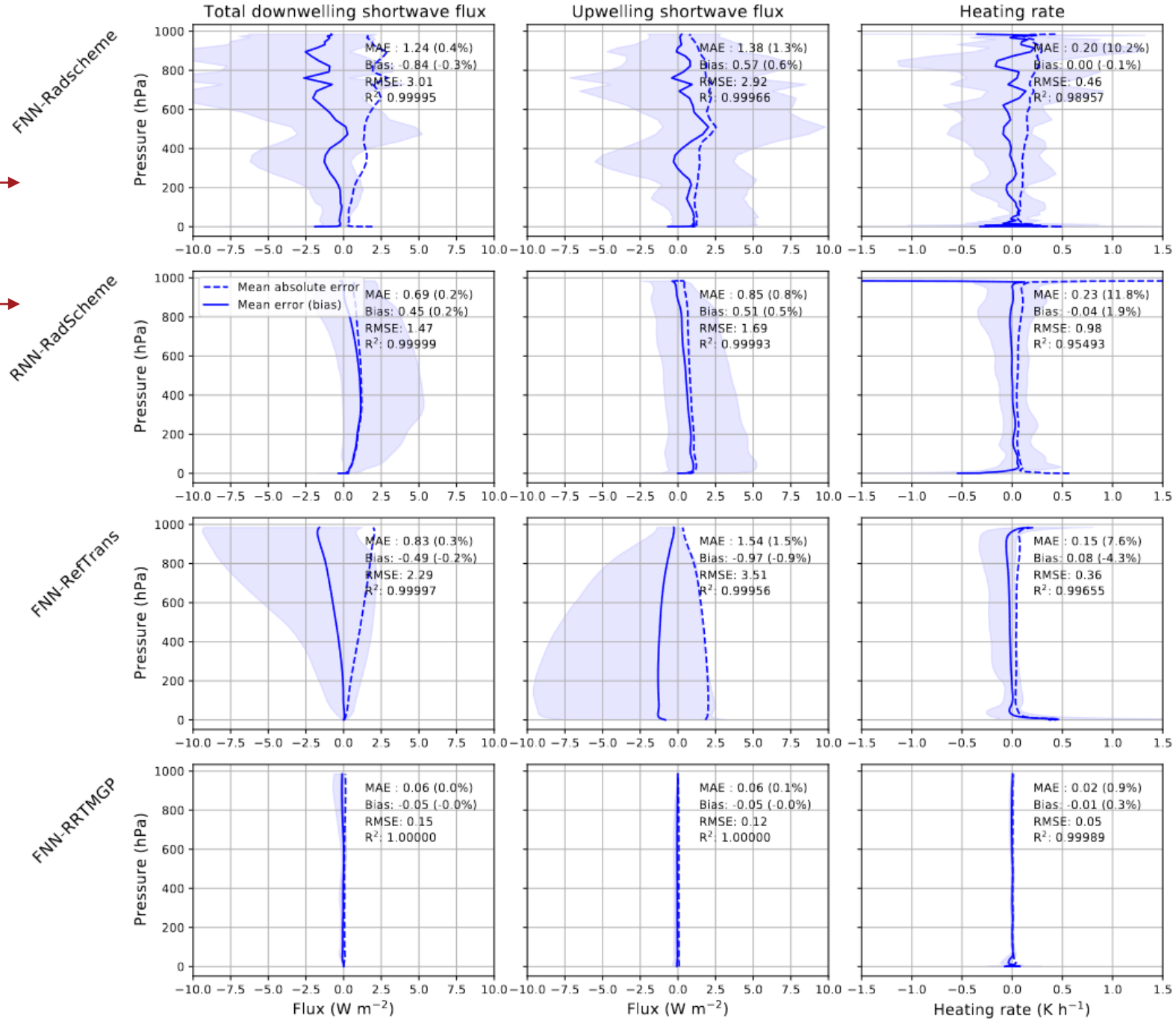
CPU: Ryzen 2600, 6 cores
GPU: GTX 1070 (no tensor cores!)

Bonus slide – UNPUBLISHED RESULTS

NN Emulation of entire radiation scheme

NN Emulation of one component in the solver (reflectance-transmittance)

NN Emulation of gas optics



Take-home message

- Climate and weather models make poor use out of modern computer hardware
- NNs can be faster than traditional parameterizations, but focusing on less exact, more empirical components may give good results mor easily
- Refactoring existing codes could also go a long way
- We combined the two to speed up a new radiation scheme by ~3x on CPUs and GPUs, seemingly without losing accuracy
- RTE+RRTMGP-NN is designed to be a usable replacement of the original code

For any questions, feel free to

- Read our paper : Ukkonen, P., Pincus, R., Hogan, R. J., Pagh Nielsen, K., & Kaas, E. (2020). Accelerating radiation computations for dynamical models with targeted machine learning and code optimization. *Journal of Advances in Modeling Earth Systems*, *12*(12)

- Check out the code at https://github.com/peterukk/rte-rrtmgp-nn
- Email me (peterukk@gmail.com / puk@dmi.dk)

ESCAPE-2: Energy-efficient SCalable Algorithms for weather and climate Prediction at Exascale

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3) Cotronei, A., & Slawig, T. (2020). Single-precision arithmetic in ECHAM radiation reduces runtime and energy consumption. https://doi.org/10.5194/gmd-13-2783-2020
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