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From Control-Centric Programming to Data-Centric Optimization





Fortran with CLOUDSC

```

9
10  SUBROUTINE CLOUDSC &
11    !---input
12    & (KIDIA,    KFDIA,    KLON,    KLEV, &
13    & PTSPHY,&
14    & PT, PQ, tendency_cml,tendency_tmp,tendency_loc, &
15    & PVFA, PVFL, PVFI, PDYNA, PDYNL, PDYNI, &
16    & PHRSW,    PHRLW,&
17    & PVERVEL,  PAP,      PAPH,&
18    & PLSM,    LDCUM,    KTYPE, &
19    & PLU,     PLUDE,    PSNDE,    PMFU,    PMFD,&
20    !---prognostic fields
21    & PA,&
22    & PCLV,  &
23    & PSUPSAT,&
24    !-- arrays for aerosol-cloud interactions
25    !!! & PQAER,    KAER, &
26    & PLCRIT_AER,PICRIT_AER,&
27    & PRE_ICE,&
28    & PCCN,     PNICE,&
29    !---diagnostic output
30    & PCOVPTOT, PRAINFRAC_TOPRFZ,&
31    !---resulting fluxes
32    & PFSQLF,   PFSQIF ,  PFCQNG,  PFCQLNG,&
33    & PFSQRF,   PFSQSF ,  PFCQRNG,  PFCQSNG,&
34    & PFSQLTUR, PFSQITUR , &
35    & PFPLSL,   PFPLSN,   PFHPSL,   PFHPSN, KFLDX, &
36    & YDCST, YDTHF, YDECLDP)

```

- **Cloud Microphysics of IFS**
 - Resolve sub-grid features
 - Original 2,525 SLOC of Fortran 95

- **Rewritten for performance portability benchmarking (optimization took months!)**
 - 2,635 SLOC C
 - 2,610 SLOC C++/CUDA

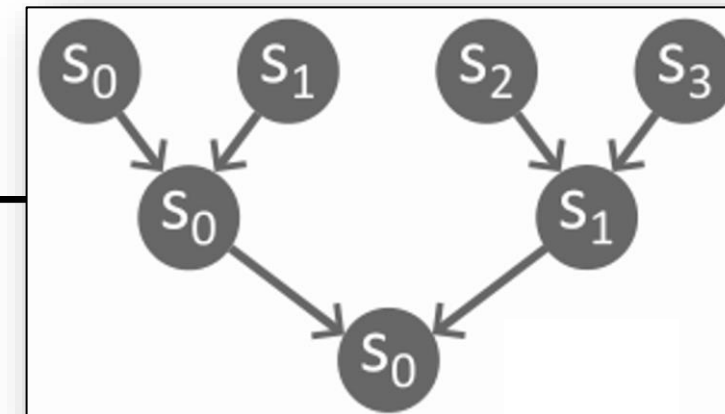
<https://github.com/ecmwf-ifs/dwarf-p-cloudsc>

A first simple loop from CLOUDSC*

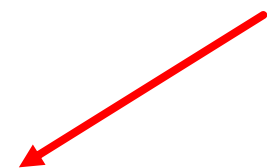
Data Parallelism	<div> <div>✓</div> <div>.....</div> <div>do JK=1,KLEV</div> </div> <div> <div>✓</div> <div>.....</div> <div>do JL=1,KFDIA</div> </div> <div> <div>ZQSM(JL,JK)=ZQSM(JL,JK)/(1.0-RE*ZQSM(JL,JK))</div> <div>enddo</div> <div>enddo</div> </div> <div>Fully data parallel</div>
Work	KLEV * KFDIA
Depth	1
Average Parallelism	KLEV * KFDIA

* examples are simplified for presentation purposes

A second more complex loop from CLOUDSC



(array) accumulation
prevents parallelization ☹️



Data Parallelism	<div> <div> <div>X</div> <div>.....</div> <div>do JN=1, NSTEP-1</div> </div> <div> <div>✓</div> <div>.....</div> <div>do JL=1, KFDIA</div> <div> $ZQXN(JL, NSTEP) = ZQXN(JL, NSTEP) + ZQXN(JL, JN)$ </div> <div>enddo</div> <div>enddo</div> </div> </div>	
Work	(NSTEP-1) * KFDIA	(NSTEP-1) * KFDIA
Depth	(NSTEP-1) * KFDIA	$\log_2(NSTEP-1)$
Average Parallelism	1	$(NSTEP-1) * KFDIA / \log_2(NSTEP-1)$

Now multiple realistic CLOUDSC loops

Data Parallelism		reuse of temporary variable prevents parallelization			Order Constraints → Happens-before	
L1	<div>X.....do JM=1,4 X.....do JK=1,KLEV X.....do JL=1,KFDIA</div>	<div>① if ZQX(JL,JK,JM)<RLMIN) then ② ZQADJ=ZQX(JL,JK,JM)*ZQTMST ③ tend_q(JL,JK)=tend_q(JL,JK)+ZQADJ ④ tend_T(JL,JK)=tend_T(JL,JK)-RAL*ZQADJ ⑤ ZQX(JL,JK,JM)=0.0</div>			<div>①→② Control ②→③ RAW ②→④ RAW ②→⑤ WAR</div>	
L2	<div>✓.....do JK=1,KLEV ✓.....do JL=1,KFDIA</div>	<div>⑥ ZQSM(JL,JK)=ZQSM(JL,JK)/(1.0-RE*ZQSM(JL,JK))</div>			<div>No order constraint L2 L1</div>	
L3	<div>✓.....do JK=1,KLEV ✓.....do JL=1,KFDIA</div>	<div>⑦ ZA(JL,JK)=MAX(0.0,MIN(1.0,ZA(JL,JK))) ⑧ ZLI(JL,JK)=ZQX(JL,JK,1)+ZQX(JL,JK,2) ⑨ if (ZLI(JL,JK)>RLMIN) then ⑩ ZLFRAC(JL,JK)=ZQX(JL,JK,1)/ZLI(JL,JK) else ⑪ ZLFRAC(JL,JK)=0.0</div>			<div>⑤→⑧ RAW ⑧→⑨ RAW ⑨→⑩ Control ⑨→⑪ Control L3 → L1</div>	
Work		4 * KLEV * KFDIA * (1+4)		KLEV * KFDIA		L1 KLEV * KFDIA * 25
Depth	L1	log2(4) * 1 * 1 * (1+2)	L2	1	L3	L2 8
Average Parallelism		KLEV * KFDIA * 10/3		KLEV * KFDIA		L3 KLEV * KFDIA * 25/8

Transformations in DaCe – Performance Metaprogramming!

Expose parallelism

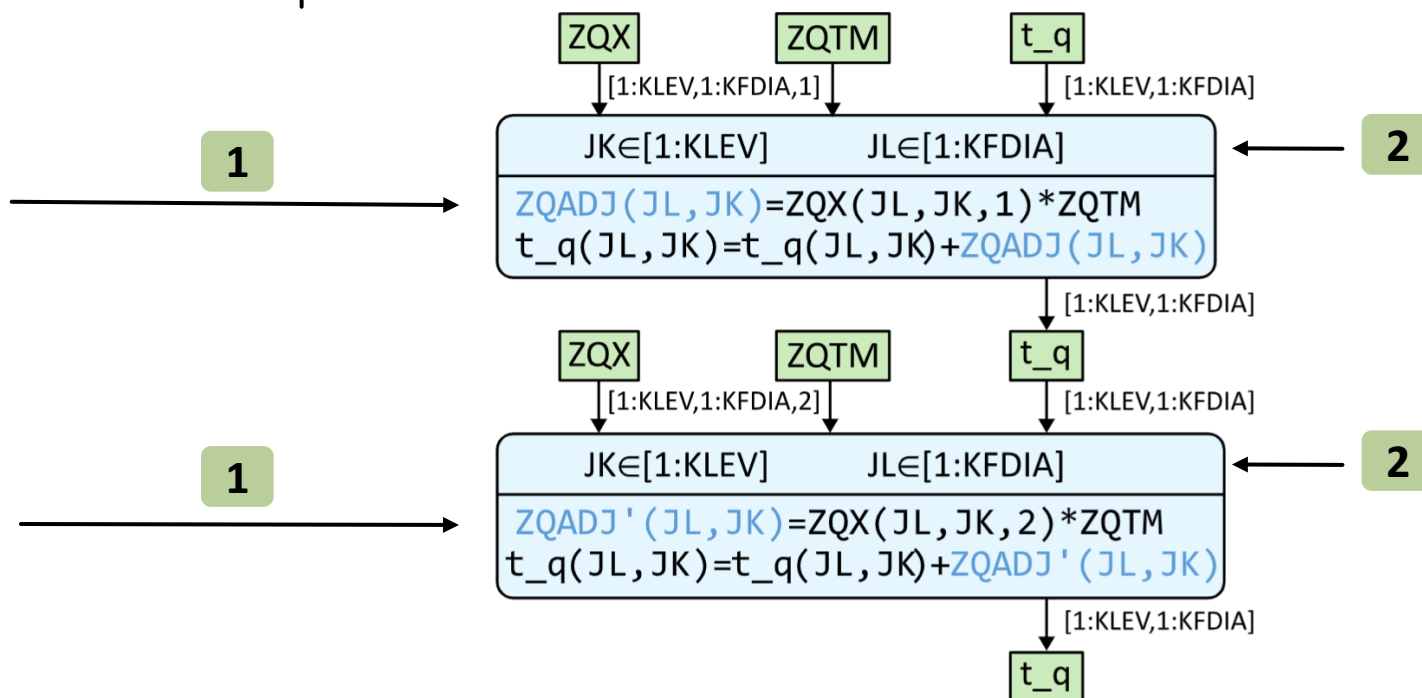
- **Data management transformations:**
 - Changing data container lifetime 1
 - Versioning data containers
- **Loop Parallelization** 2

```
do JK=1,KLEV
  do JL=1,KFDIA
    ZQADJ=ZQX(JL,JK,1)*ZQTM
    t_q(JL,JK)=t_q(JL,JK)+ZQADJ
  enddo
enddo
```

```
do JK=1,KLEV
  do JL=1,KFDIA
    ZQADJ=ZQX(JL,JK,2)*ZQTM
    t_q(JL,JK)=t_q(JL,JK)+ZQADJ
  enddo
enddo
```

Improve performance

- **Specializing numerical values**
- **Changing the data layout**



Minimizing depth!

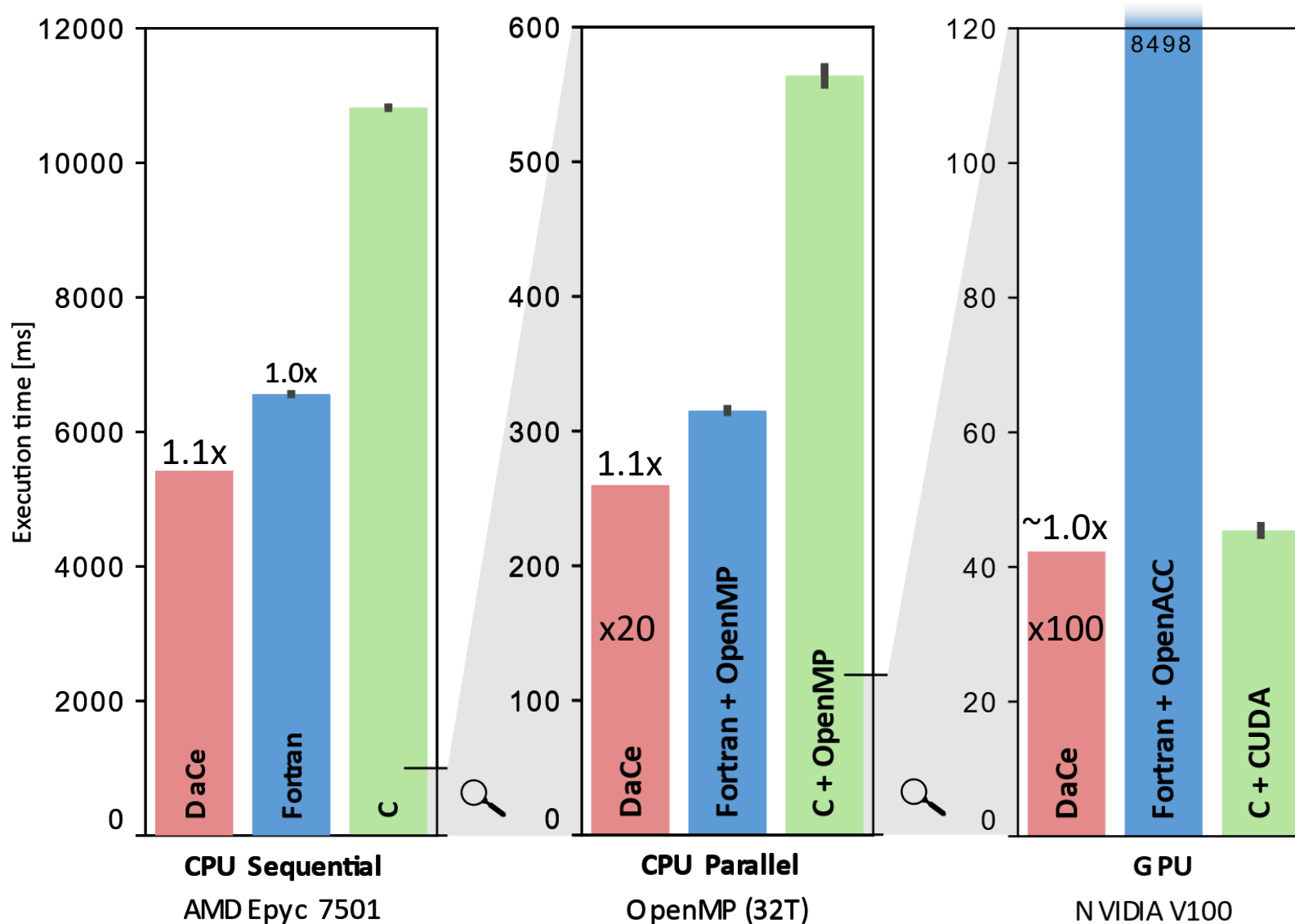
```
! Function Definitions
REAL :: FOEEWM, FOELDCPM
FOEEWM ( PTARE ) = R2ES * &
  &(MIN(1.0, ((MAX(RTICE, MIN(RTWAT, PTARE)) - RTICE) * RTWAT_RTICE_R)**2) &
  & * EXP(R3LES * (PTARE - RTT) / (PTARE - R4LES)) &
  & + (1.0 - MIN(1.0, ((MAX(RTICE, MIN(RTWAT, PTARE)) - RTICE) * RTWAT_RTICE_R)**2)) &
  & * EXP(R3IES * (PTARE - RTT) / (PTARE - R4IES)))
FOELDCPM ( PTARE ) = MIN(1.0, ((MAX(RTICE, MIN(RTWAT, PTARE)) - &
  & RTICE) * RTWAT_RTICE_R)**2) * RALVDCP + &
  & (1.0 - MIN(1.0, ((MAX(RTICE, MIN(RTWAT, PTARE)) - RTICE) * RTWAT_RTICE_R)**2)) * RALSDCP

! Vertical loop
DO JK=NCLDTP, KLEV
...
  ! Loop Nest
  DO JL=KIDIA, KFDIA
    ZQP = 1.0/PAP(JL, JK)
    ZQSAT = FOEEWM(ZTP1(JL, JK)) * ZQP
    ZQSAT = MIN(0.5, ZQSAT)
    ZCOR = 1.0/(1.0 - RETV * ZQSAT)
    ZQSAT = ZQSAT * ZCOR
    ZCOND = (ZQSMIX(JL, JK) - ZQSAT) / (1.0 + ZQSAT * ZCOR * FOEDEM(ZTP1(JL, JK)))
    ZTP1(JL, JK) = ZTP1(JL, JK) + FOELDCPM(ZTP1(JL, JK)) * ZCOND
    ZQSMIX(JL, JK) = ZQSMIX(JL, JK) - ZCOND
    ZQSAT = FOEEWM(ZTP1(JL, JK)) * ZQP
    ZQSAT = MIN(0.5, ZQSAT)
    ZCOR = 1.0/(1.0 - RETV * ZQSAT)
    ZQSAT = ZQSAT * ZCOR
    ZCOND1 = (ZQSMIX(JL, JK) - ZQSAT) / (1.0 + ZQSAT * ZCOR * FOEDEM(ZTP1(JL, JK)))
    ZTP1(JL, JK) = ZTP1(JL, JK) + FOELDCPM(ZTP1(JL, JK)) * ZCOND1
    ZQSMIX(JL, JK) = ZQSMIX(JL, JK) - ZCOND1
  ENDDO
...
ENDDO
```

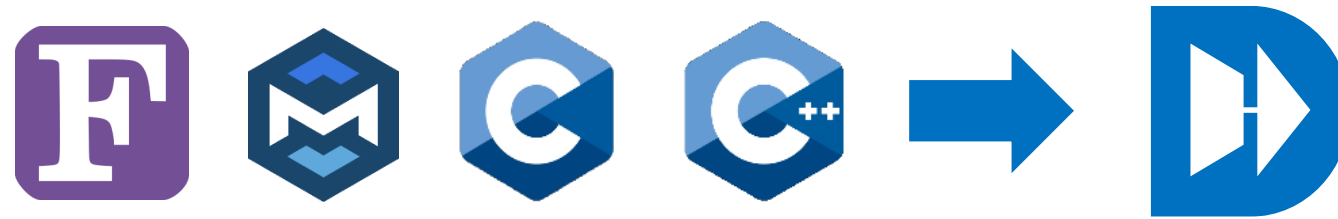


```
...
! Vertical loop
DO JK=NCLDTP, KLEV
...
  ! Loop Nest
  DO JL=KIDIA, KFDIA
    ZQP_0(JL) = 1.0/PAP(JL, JK)
  ENDDO
  DO JL=KIDIA, KFDIA
    ZQSAT = FOEEWM(ZTP1(JL, JK)) * ZQP_0(JL)
    ZQSAT = MIN(0.5, ZQSAT)
    ZCOR = 1.0/(1.0 - RETV * ZQSAT)
    ZQSAT = ZQSAT * ZCOR
    ZCOND_0(JL) = (ZQSMIX(JL, JK) - ZQSAT) / (1.0 + ZQSAT * ZCOR * FOEDEM(ZTP1(JL, JK)))
  ENDDO
  DO JL=KIDIA, KFDIA
    ZTP1(JL, JK) = ZTP1(JL, JK) + FOELDCPM(ZTP1(JL, JK)) * ZCOND_0(JL)
  ENDDO
  DO JL=KIDIA, KFDIA
    ZQSMIX(JL, JK) = ZQSMIX(JL, JK) - ZCOND_0(JL)
  ENDDO
  DO JL=KIDIA, KFDIA
    ZQSAT = FOEEWM(ZTP1(JL, JK)) * ZQP_0(JL)
    ZQSAT = MIN(0.5, ZQSAT)
    ZCOR = 1.0/(1.0 - RETV * ZQSAT)
    ZQSAT = ZQSAT * ZCOR
    ZCOND1_0(JL) = (ZQSMIX(JL, JK) - ZQSAT) / (1.0 + ZQSAT * ZCOR * FOEDEM(ZTP1(JL, JK)))
  ENDDO
  DO JL=KIDIA, KFDIA
    ZTP1(JL, JK) = ZTP1(JL, JK) + FOELDCPM(ZTP1(JL, JK)) * ZCOND1_0(JL)
  ENDDO
  DO JL=KIDIA, KFDIA
    ZQSMIX(JL, JK) = ZQSMIX(JL, JK) - ZCOND1_0(JL)
  ENDDO
...
ENDDO
```

Performance portability – all from the original, unchanged CLOUDSC code!



Conclusion



Canonicalization is key to performance & portability