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# Introduction to High-Performance Computing

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# Agenda

- ✓ **HPC: What is it?**
  - ✓ **Hardware: how it works**
  - ✓ **Algorithm vs. Implementation**
  - ✓ **Compiler + Floating point + I/O**
  - ✓ Parallel Paradigm
  - ✓ Conclusions & Comments
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# HPC: what it is?

- ✓ These are the main skills for an efficient HPC



# Which programming language?

[https://en.wikipedia.org/wiki/List\\_of\\_programming\\_languages](https://en.wikipedia.org/wiki/List_of_programming_languages)

✓ 690 different programming languages

- TeX
- Postscript
- C- -
- [Ballerina](#)
- [Mystic Programming Language \(MPL\)](#)

## List of programming languages

[Article](#) [Talk](#)

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This is an index to notable [programming languages](#), in current or historical use. [Dialects](#) of [BASIC](#), [esoteric programming languages](#), and [markup languages](#) are not included. A programming language does not need to be [imperative](#) or [Turing-complete](#), but must be [executable](#) and so does not include [markups](#) such as [HTML](#) or [XML](#), but does include [domain-specific languages](#) such as [SQL](#) and its [dialects](#).

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<ul style="list-style-type: none"><li>• <a href="#">A.NET (A#/A sharp)</a></li><li>• <a href="#">A-0 System</a></li><li>• <a href="#">A+ (A plus)</a></li><li>• <a href="#">ABAP</a></li><li>• <a href="#">ABC</a></li><li>• <a href="#">ABC ALGOL</a></li><li>• <a href="#">ACC</a></li><li>• <a href="#">Accent (Rational Synergy)</a></li><li>• <a href="#">Ace Distributed Application Specification</a></li></ul>	<ul style="list-style-type: none"><li>• <a href="#">Agilent VEE (Keysight VEE)</a></li><li>• <a href="#">Agora</a></li><li>• <a href="#">AIMMS</a></li><li>• <a href="#">Aldor</a></li><li>• <a href="#">Alef</a></li><li>• <a href="#">ALF</a></li><li>• <a href="#">ALGOL 58</a></li><li>• <a href="#">ALGOL 60</a></li><li>• <a href="#">ALGOL 68</a></li></ul>	<ul style="list-style-type: none"><li>• <a href="#">Apache Pig latin</a></li><li>• <a href="#">Apex (Salesforce.com, Inc)</a></li><li>• <a href="#">APL</a></li><li>• <a href="#">App Inventor for Android's visual block language (MIT App Inventor)</a></li><li>• <a href="#">AppleScript</a></li><li>• <a href="#">APT</a></li><li>• <a href="#">Arc</a></li><li>• <a href="#">ARexx</a></li></ul>
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# Programming Languages

- ✓ A **compiled language** is a programming language whose implementations pass through a compiler. It is a translator that generates machine code from source code
    - e.g. Fortran, C, C++, ...
    - Syntax must be correct before running
    - Can be optimized by the compiler
  - ✓ An **interpreted language** is a programming language that is executed step-by-step, with no pre-runtime translation
    - E.g. Perl, Python, bash, ....
    - It runs until it finds a syntax error
    - Optimization usually could be very low
-

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# Compiler: how it works?

***compiler** is a computer program that translates computer code written in one programming language (the source language) into another language (the target language). The name "compiler" is primarily used for programs that translate source code from a high-level programming language to a low-level programming language (e.g. assembly language, object code, or machine code) to create an executable program*

## **1. Front-End**

- a. Pre-processing
- b. Syntax & Semantic check/analysis

## **2. Middle-End**

- a. (general) Optimization

## **3. Back-End**

- a. Machine dependent optimization
  - b. Code Generation
-

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# Compiler: Optimization level

Have you ever read compiler's manual?

What the different level of optimization means? For `nvfortran` compiler

- ✓ **-O**: All -O1 optimizations plus traditional global scalar optimizations performed
  - ✓ **-O0**: Creates a basic block for each statement. No scheduling or global optimizations performed
  - ✓ **-O1**: Some scheduling and register allocation is enabled. No global optimizations performed
  - ✓ **-O2**: All -O optimizations plus SIMD code generation. Implies -Mvect=simd
  - ✓ **-O3**: All -O2 optimizations plus more aggressive code hoisting and scalar replacement, that may or may not be profitable, Implies -Mvect=simd
  - ✓ **-O4**: All -O3 optimizations plus more aggressive hoisting of guarded expressions performed. Implies -Mvect=simd
  - ✓ **-fast**: Common optimizations; includes -O2 -Munroll=c:1 -Mlre -Mautoinline, Implies -Mvect=simd -Mflushz -Mcache\_align
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## Optimization level example: MMM

- ✓ Different level of optimization for size=1000 matrices (on different machine)

Opzione	IBM xlf (sec.)	HP f77 (sec.)	Portland pgf77 (sec.)
-00	176	185	32.0
-01	-	237	30.9
-02	121	115	29.6
-03	122	98.1	-
-04	3.1	98.4	-
-05	3.8	4.9	-



- ✓ Old example (IBM)
- ✓ Old but “quite” clear
- ✓ Where does this difference in time comes from?

Option	Time (sec.)
-O0	24''
-O2	6.35''
-O3	4.87''
-O4	2.14''

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# Reading the assembler

## ✓ Old example (IBM)

```
65 | do k = 1, n
66 |     do j = 1, n
67 |         do i = 1, n
68 |             c(i,j) = c(i,j) + a(i,k)*b(k,j)
69 |         enddo
70 |     enddo
71 | enddo
```

## ✓ Compiler can produce, if you activate the right flags

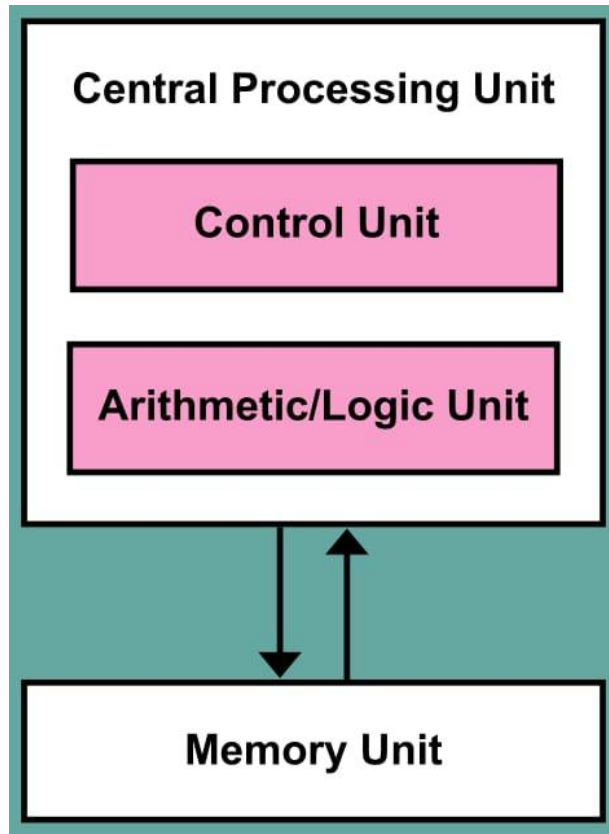
- Listing file (for IBM \*.lst)
  - Assembler file (for IBM \*.s)
-

# Recap: Von Neumann's model/load-store

- ✓ Independent Systems that talk to each other exchanging data
  - Moving data/instructions
  - Performing operations
- ✓ Data and instructions are stored in the same area
- ✓ Different, and independent, units for instructions (Control Units) and data (ALU units)

## Two key points

- ✓ Data moved back and forth from main memory
- ✓ Instructions (e.g. Flops) performed from Memory



# reading the assembler: -O0 option

✓ mm.lst

68	0004B4	lwz	80820008	1	L4A	gr4=.\$STATIC_BSS(gr2,0)
68	0004B8	lwz	80640004	2	L4A	gr3=j(gr4,4)
68	0004BC	rlwinm	54636824	2	SLL4	r3=gr3,13
68	0004C0	lwz	80A40008	1	L4A	gr5=i(gr4,8)
68	0004C4	rlwinm	54A51838	2	SLL4	gr5=gr5,3
68	0004C8	add	7CC32A14	1	A	gr6=gr3,gr5
68	0004CC	addis	3CE40100	1	AIU	gr7=gr4,256
68	0004D0	add	7CC63A14	1	A	gr6=gr6,gr7
68	0004D4	lfd	C826E018	1	LFL	fp1=c[](gr6,-8168)
68	0004D8	lwz	80C40010	1	L4A	gr6=k(gr4,16)
68	0004DC	rlwinm	54C76824	2	SLL4	gr7=gr6,13
68	0004E0	add	7CE53A14	1	A	gr7=gr5,gr7
68	0004E4	add	7CE43A14	1	A	gr7=gr4,gr7
68	0004E8	lfd	C847E018	1	LFL	fp2=a[](gr7,-8168)

...

## reading the assembler: -O0 option

```
...
68 | 0004EC    rlwinm    54C61838    1    SLL4    gr6=gr6,3
68 | 0004F0    add       7CE33214    1    A       gr7=gr3,gr6
68 | 0004F4    addis     3CC40080    1    AIU     gr6=gr4,128
68 | 0004F8    add       7CC63A14    1    A       gr6=gr6,gr7
68 | 0004FC    lfd        C866E018    1    LFL     fp3=b[] (gr6,-8168)
68 | 000500    fmadd      FC2208FA    1    FMA     fp1=fp1-fp3,fcr
68 | 000504    add       7C632A14    0    A       gr3=gr3,gr5
68 | 000508    addis     3C840100    1    AIU     gr4=gr4,256
68 | 00050C    add       7C632214    1    A       gr3=gr3,gr4
68 | 000510    stfd      D823E018    1    STFL    c[] (gr3,-8168)=fp1
```

- ✓ mm.lst: 24 instructions but
- only 1 store
  - only 3 load
  - only 1 fused-multiply and add (i.e. 2 flops)
  - → 2/24 peak performance (~8%)

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## reading the assembler: -O0 option

- ✓ mm.lst: 24 instructions but
    - only 1 store
    - only 3 load
    - only 1 fused-multiply and add (i.e. 2 flops)
    -
  - ✓ Other 19 instructions where do they come from?
- 
- ✓ Integer operation to compute address (i.e. element location in memory)
  - ✓ 19/24 of total instructions “spent” in understanding where data is!!!
  - ✓ ~80% of total time only to “understand”, data fetching could be more expensive (e.g. cache miss)
-

## reading the assembler: -O2 option

✓ mm.lst

```
68 | 0003D8 lfd C8070008 1 LFL fp0=c (gr7,8)
0 | 0003DC mtspr 7F8903A6 1 LCTR ctr=gr28
0 | 0003E0 ori 63080000 1 LR gr8=gr24
0 | 0003E4 lfdu CC662000 1 LFDU fp3,gr6=b (gr6,8192)
0 | 0003E8 ori 60E90000 1 LR gr9=gr7
68 | 0003EC lfdu CC280008 1 LFDU fp1,gr8=a (gr8,8)
68 | 0003F0 fmadd FC0100FA 1 FMA fp0=fp0,fp1,fp3,fc
0 | 0003F4 bc 43400018 0 BCF ctr=CL.111,taken=0%(0,100)
68 | 0003F8 lfd C8490010 1 LFL fp2=c (gr9,16)
68 | 0003FC lfdu CC280008 1 LFDU fp1,gr8=a (gr8,8)
68 | 000400 stfdu DC090008 1 STFDU gr9,c (gr9,8)=fp0
68 | 000404 fmadd FC0110FA 1 FMA fp0=fp2,fp1,fp3,fc
0 | 000408 bc 4320FFF0 0 BCT ctr=CL.29,taken=100%(100,0)
0 | CL.111:
68 | 000410 stfdu DC09000 1 STFDU gr9,c (gr9,8)=fp0
```

...

# reading the assembler: -O2 option

- ✓ mm.lst: 15 instructions
  - 2 store
  - 5 load
  - 2 fused-multiply and add
  - → 4/15 peak performance (~26%)

✓ mm.s

```
__L3d8:                                # 0x000003d8 (H.10.NO_SYMBOL+0x3d8)
    lfd    fp0,8(r7)
    mtspr   CTR,r28
    oril    r8,r24,0x0000
    lfd    fp3,8192(r6)
    oril    r9,r7,0x0000
    lfd    fp1,8(r8)
    fma     fp0,fp1,fp3,fp0
    .machine "any"
    bc     B0_dCTR_ZERO_8,CRO_LT,__L40c
__L3f8:                                # 0x000003f8 (H.10.NO_SYMBOL+0x3f8)
    lfd     fp2,16(r9)
    lfd     fp1,8(r8)
    stfdu   fp0,8(r9)
    fma     fp0,fp1,fp3,fp2
    bc     B0_dCTR_NZERO_9,CRO_LT,__L3f8
```



## reading the assembler: -O3 option

✓ mm.lst

68	000478	lfd	C8910008	1	LFL	fp4=a (gr17,8)
0	00047C	mtspr	7D0903A6	1	LCTR	ctr=gr8
0	000480	ori	62260000	1	LR	gr6=gr17
0	000484	lfdu	CC042000	1	LFDU	fp0,gr4=b (gr4,8192)
0	000488	ori	60A70000	1	LR	gr7=gr5
68	00048C	lfd	C8650008	1	LFL	fp3=c (gr5,8)
68	000490	lfd	C8D10010	1	LFL	fp6=a (gr17,16)
68	000494	lfd	C8E50010	1	LFL	fp7=c (gr5,16)
68	000498	lfd	C8310018	1	LFL	fp1=a (gr17,24)
68	00049C	lfdu	CCA60020	1	LFDU	fp5,gr6=a (gr6,32)
68	0004A0	lfd	C8450018	1	LFL	fp2=c (gr5,24)
68	0004A4	fmadd	FC64183A	1	FMA	fp3=fp3,fp4,fp0, fcr
68	0004A8	lfd	C8850020	1	LFL	fp4=c (gr5,32)
68	0004AC	fmadd	FCC6383A	1	FMA	fp6=fp7,fp6,fp0, fcr
68	0004B0	bc	43400048	0	BCF	ctr=CL.126,taken=0%(0,100)
68		CL.127:				
68	0004B4	fmadd	FC21103A	1	FMA	fp1=fp2,fp1,fp0, fcr

## reading the assembler: -O3 option

✓ mm.lst

68	0004B8	stfd	D8670008	1	STFL	c (gr7,8)=fp3
68	0004BC	lfd	C8470028	1	LFL	fp2=c (gr7,40)
68	0004C0	stfd	D8C70010	1	STFL	c (gr7,16)=fp6
68	0004C4	lfd	C8660008	1	LFL	fp3=a (gr6,8)
68	0004C8	fmadd	FC85203A	1	FMA	fp4=fp4,fp5,fp0, fcr
68	0004CC	lfd	C8A70030	1	LFL	fp5=c (gr7,48)
68	0004D0	lfd	C8C60010	1	LFL	fp6=a (gr6,16)
68	0004D4	stfd	D8270018	1	STFL	c (gr7,24)=fp1
68	0004D8	fmadd	FC63103A	1	FMA	fp3=fp2,fp3,fp0, fcr
68	0004DC	lfd	C8470038	1	LFL	fp2=c (gr7,56)
68	0004E0	lfd	C8260018	1	LFL	fp1=a (gr6,24)
68	0004E4	fmadd	FCC6283A	1	FMA	fp6=fp5,fp6,fp0, fcr
68	0004E8	stfdu	DC870020	1	STFDU	gr7, c (gr7,32)=fp4
68	0004EC	lfd	C8870020	1	LFL	fp4=c (gr7,32)
68	0004F0	lfdu	CCA60020	1	LFDU	fp5,gr6=a (gr6,32)
0	0004F4	bc	4320FFC0	0	BCT	ctr=CL.127,taken=100%(100,0)
68			CL.126:			

## reading the assembler: -O3 option

- ✓ mm.lst: 34 instructions
  - 4 store
  - 16 load
  - 6 fused-multiply and add
  - → 12/34 peak performance (~35%)

✓ mm.s

```
lfd      fp4,8(r17)
mtspr    CTR,r8
oril      r6,r17,0x0000
lfd      fp0,8192(r4)
oril      r7,r5,0x0000
lfd      fp3,8(r5)
lfd      fp6,16(r17)
lfd      fp7,16(r5)
lfd      fp1,24(r17)
lfd      fp5,32(r6)
lfd      fp2,24(r5)
fma      fp3,fp4,fp0,fp3
lfd      fp4,32(r5)
fma      fp6,fp6,fp0,fp7
```

---

## reading the assembler: -O5 option

- ✓ mm.lst: 344 instructions
    - 64 store
    - 128 load
    - 100 fused-multiply and add
    - → 200/344 peak performance (~58%)
    - → unrolling outer loop
    - → blocking
-

- ✓ Old example (IBM pwr)
- ✓ Old but quite clear
- ✓ Now we know where these figures comes from

Option	Time (sec.)	%flops instructions
-O0	24''	8%
-O2	6.35''	26%
-O3	4.87''	37%
-O4	2.14''	58%

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# Compiler: what it can do?

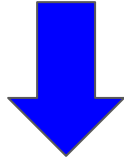
Many optimization:

- ✓ Dead and redundant code removal
  - ✓ Copy propagation
  - ✓ Code motion
  - ✓ Strength reduction
  - ✓ Common subexpression elimination
  - ✓ Register allocation
  - ✓ Loop pipelining/unrolling
  - ✓ Cache blocking
  - ✓ Loop interchange/reordering
  - ✓ Function inlining
  - ✓ ....
-

# Code Motion

- ✓ A compiler can move instructions (e.g. outside of a loop) only if it realizes that the result is not affected by this transformation

```
do i = 1, n
  somma = somma + a(i)*b(j)*c(k)
enddo
```



```
temp = b(j)*c(k)
do i = 1, n
  somma = somma + a(i)*temp
enddo
```

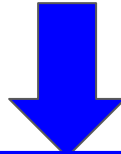
```
do i = 1, n
  somma = somma + (a(i)*b(j))*c(k)
enddo
```

---

# Common Subexpression Elimination

- ✓ A compiler can group operations to reduce total number of instructions

```
x = c*sin(a)*cos(b)
y = c*sin(a)*sin(b)
x = c*cos(a)
```



```
temp = c*sin(a)
x = temp*cos(b)
y = temp*sin(b)
z = c*cos(a)
```

---



# Strength Reduction

- ✓ Math Functions can be very expensive
- ✓ the compiler can change one operation with another equivalent one but less expensive
  - $a^{**2} \rightarrow a*a$
- ✓ but only at high level of optimization
- ✓ or use fast math libraries
  - but result can be different  $\rightarrow$  Finite precision

Function	Cycles
<b>sin(x)</b>	230
<b>exp(x)</b>	535
<b>log(x)</b>	423
<b>acos(x)</b>	635
<b>x**1.5</b>	945
<b>x**2</b>	27
<b>sqrt(x)</b>	54
<b>x**2.0</b>	674
<b>1/x</b>	50

---

# inlining

***inline expansion**, or **inlining**, is a manual or compiler optimization that replaces a function call site with the body of the called function. Inline expansion is similar to macro expansion, but occurs during compilation, without changing the source code (the text), while macro expansion occurs prior to compilation, and results in different text that is then processed by the compiler.*

- ✓ The code is less compact and more verbose
- ✓ All overhead of function is removed, allowing further optimization
- ✓ profiling can help to spot fast functions
  - → `gprof`

## inlining: example

- ✓ The code is less compact and more verbose
- ✓ Overheads of function are removed, allowing further optimization (e.g. unrolling)

```
do i = 1, n
  .....
  call somma(a,b,c)
  .....
enddo

subroutine somma
real a,b,c
c = c + a*b
return
```



```
do i = 1, n
  .....
  c = c + a*b
  .....
enddo
```

# Loop reordering

- ✓ Using high optimization levels, the compiler “can” reorder loops to make it more efficient (i.e. cache efficient)
- ✓ But it can be confused by
  - Coding style
  - pointers
  - functions inside the loop
  - too much nested loops
  - I/O statements

```
72 do i = 1, n
73     do k = 1, n
74         do j = 1, n
75             c(i,j) = c(i,j) + a(i,k)*b(k,j)
76         enddo
77     enddo
78 enddo
```

# Loop reordering: example

✓ 2048 Matrix size: 114" (-O0) vs. 3.3" (-O3)

```
gamati01@dgx03:/$ nvfortran -O0 -Minfo mm.F90 mod_tools.F90 -o mm.slow
mm.F90:
mm:
    75, FMA (fused multiply-add) instruction(s) generated
```

```
gamati01@dgx03:/$ nvfortran -O3 -Minfo mm.F90 mod_tools.F90 -o mm.fast
mm.F90:
mm:
    64, Memory zero idiom, array assignment replaced by call to pgf90_mzero8
    72, Loop interchange produces reordered loop nest: 74,73,72
        Generated vector simd code for the loop
    73, Zero trip check eliminated
    74, Zero trip check eliminated
        Loop not fused: function call before adjacent loop
    75, FMA (fused multiply-add) instruction(s) generated
```

# Loop reordering

- ✓ Too much loops can confuse the compiler
- ✓ Remember: compilers are “conservative”. They do not perform optimization unless they are sure of having no side effects!

```
81 do ii = 1, n, step
82     do kk = 1, n, step
83         do jj = 1, n, step
84             do j = jj, jj+step-1
85                 do k = kk, kk+step-1
86                     do i = ii, ii+step-1
87                         c(i,j) = c(i,j) + a(i,k)*b(k,j)
88                     enddo
89                 enddo
90             enddo
91         enddo
92     enddo
93 enddo
```

# Loop reordering: example

✓ 4096 Matrix size: 384" (-O0) vs. 19.1" (-O3) vs 11.1" (-O3, correct loop ordering)

```
gamati01@dgx03:/$ nvfortran -O0 -Minfo mm.F90 mod_tools.F90 -o mm.slow
mm:
    75, FMA (fused multiply-add) instruction(s) generated
```

```
gamati01@dgx03:$ nvfortran -O3 -Minfo mm.F90 mod_tools.F90 -o mm.fast
mm:
    73, Memory zero idiom, array assignment replaced by call to pgf90_mzero8
    81, Loop not fused: function call before adjacent loop
        Loop not vectorized/parallelized: too deeply nested
    82, Loop not vectorized/parallelized: too deeply nested
    83, Loop not vectorized/parallelized: too deeply nested
    85, Zero trip check eliminated
    86, Zero trip check eliminated
        Generated vector simd code for the loop
    87, FMA (fused multiply-add) instruction(s) generated
```

---

## pointers: an example

### Kinetic code

- ✓ Using pointer to “swap” arrays: current → old

```
real(mystorage), dimension(:,:,:), pointer :: a01,a02,a03,a04,a05
real(mystorage), dimension(:,:,:), pointer :: a06,a07,a08,a09,a10
real(mystorage), dimension(:,:,:), pointer :: a11,a12,a13,a14,a15
real(mystorage), dimension(:,:,:), pointer :: a16,a17,a18,a19
!
real(mystorage), dimension(:,:,:), pointer :: b01,b02,b03,b04,b05
real(mystorage), dimension(:,:,:), pointer :: b06,b07,b08,b09,b10
real(mystorage), dimension(:,:,:), pointer :: b11,b12,b13,b14,b15
real(mystorage), dimension(:,:,:), pointer :: b16,b17,b18,b19
```



## pointers: an example

```
nvfortran -DPGI -O2 -Mnodepchk -DFUSED -c col_MC.F90
```

```
...
```

Mean	time	0.800468E-01	100/	20000
Mean	time	0.811069E-01	200/	20000
Mean	time	0.819973E-01	300/	20000
Mean	time	0.813246E-01	400/	20000
Mean	time	0.807486E-01	500/	20000

```
...
```

```
nvfortran -DPGI -O2 -Mnodepchk -Mcontiguous -DFUSED -c col_MC.F90
```

```
...
```

Mean	time	0.426128E-01	100/	20000
Mean	time	0.425005E-01	200/	20000
Mean	time	0.423607E-01	300/	20000
Mean	time	0.424811E-01	400/	20000
Mean	time	0.421280E-01	500/	20000

```
...
```

## pointers: language can help!

- ✓ Fortran2008 has an attribute for contiguous pointers to leverage compiler's efforts.

```
real(mystorage), dimension(:,:,:), contiguous, pointer :: a01,a02,a03,a04,a05  
real(mystorage), dimension(:,:,:), contiguous, pointer :: a06,a07,a08,a09,a10  
real(mystorage), dimension(:,:,:), contiguous, pointer :: a11,a12,a13,a14,a15  
real(mystorage), dimension(:,:,:), contiguous, pointer :: a16,a17,a18,a19
```

```
nvfortran -DPGI -O2 -Mnodepchk -DFUSED -c col_MC.F90
```

...

Mean	time	0.430257E-01	100/	20000
Mean	time	0.431001E-01	200/	20000
Mean	time	0.431249E-01	300/	20000
Mean	time	0.431014E-01	400/	20000
Mean	time	0.433579E-01	500/	20000

...

---

## Another example.....

Implementing Turbulence model  
(Smagorinsky Model) in a 3D Lattice  
Boltzmann model

$$\nu_{total} = \nu_0 + \underbrace{(C_S \Delta)^2 |S|}_{\nu_t}$$

$$S_{ij} = -\frac{3\omega_s}{2\rho_{(0)}} \Pi_{ij}^{(neq)}$$

$$\Pi_{ij}^{(neq)} = \sum_q c_{qi} c_{qj} f_q^{(neq)}$$

---

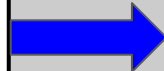
## An example.....

$$\Pi_{ij}^{(neq)} = \sum_q c_{qi} c_{qj} f_q^{(neq)}$$

- ✓ 19\*6\*2 multiplications
- ✓ 19\*6 sums
- ✓ 19\*6\*3 loads

What can a compiler do?

```
do i
  do j
    do k
      ...
      do pop=1,19
        Pxx = Pxx + cx(pop)*cx(pop)*neq(pop)
        Pyy = Pyy + cy(pop)*cy(pop)*neq(pop)
        Pzz = Pzz + cz(pop)*cz(pop)*neq(pop)
        Pxy = Pxy + cx(pop)*cy(pop)*neq(pop)
        Pxz = Pxz + cx(pop)*cz(pop)*neq(pop)
        Pyz = Pyz + cy(pop)*cz(pop)*neq(pop)
      enddo
    enddo
  enddo
enddo
...
```



## first “optimization”

$$\Pi_{ij}^{(neq)} = \sum_q c_{qi} c_{qj} f_q^{(neq)}$$

- ✓ 19\*6\*2 multiplications
- ✓ 19\*6 sums
- ✓ 19\*6\*2 loads

What can a compiler do?  
Maybe this.....



```
...  
Pxx = cx(01)*cx(01)*n01 + cx(02)*cx(02)*n02 + &  
      cx(03)*cx(03)*n03 + cx(04)*cx(04)*n04 + &  
      cx(05)*cx(05)*n05 + cx(06)*cx(06)*n06 + &  
      cx(07)*cx(07)*n07 + cx(08)*cx(08)*n08 + &  
      cx(09)*cx(09)*n09 + cx(10)*cx(10)*n10 + &  
      cx(11)*cx(11)*n11 + cx(12)*cx(12)*n12 + &  
      cx(13)*cx(13)*n13 + cx(14)*cx(14)*n14 + &  
      cx(15)*cx(15)*n15 + cx(16)*cx(16)*n16 + &  
      cx(17)*cx(17)*n17 + cx(18)*cx(18)*n18 + &  
      cx(19)*cx(19)*n19  
Pyy = cy(01)*cy(01)*n01 + cy(02)*cy(02)*n02 + &  
...  
...
```

## Some performance figures

- ✓ Left: time for  $256^3$  simulation without Smagorinsky Model
- ✓ Right: time for  $256^3$  simulation with Smagorinsky Model

# Time for section			
# init	time	0.115159E+01	
# loop	time	0.716699E+02	
# coll	time	0.641728E+02	
# bc	time	0.645609E+01	
# diagno	time	0.102584E+01	

# Time for section			
# init	time	0.111767E+01	
# loop	time	0.866046E+02	
# coll	time	0.791241E+02	
# bc	time	0.645086E+01	
# diagno	time	0.101066E+01	

- ✓ the Smagorinsky model introduce a 1.23x slowdown!
- ✓ Can it be reduced?

## Looking at operation

✓ For each Tensor element  $P_{ij}$  we perform

- 19\*3 load operation
- 19 sums
- 19\*2 products

```
Pxy = cx(01)*cy(01)*n01 + cx(02)*cy(02)*n02 + &  
      cx(03)*cy(03)*n03 + cx(04)*cy(04)*n04 + &  
      cx(05)*cy(05)*n05 + cx(06)*cy(06)*n06 + &  
      cx(07)*cy(07)*n07 + cx(08)*cy(08)*n08 + &  
      cx(09)*cy(09)*n09 + cx(10)*cy(10)*n10 + &  
      cx(11)*cy(11)*n11 + cx(12)*cy(12)*n12 + &  
      cx(13)*cy(13)*n13 + cx(14)*cy(14)*n14 + &  
      cx(15)*cy(15)*n15 + cx(16)*cy(16)*n16 + &  
      cx(17)*cy(17)*n17 + cx(18)*cy(18)*n18 + &  
      cx(19)*cy(19)*n19
```

✓ But  $cx(j)$ ,  $cy(j)$ ,  $cz(j)$  can assume only values among -1, 0, +1

- only 10 non zero values for  $cx(j)$ ,  $cy(j)$ ,  $cz(j)$

## Second optimization:

$$\Pi_{ij}^{(neq)} = \sum_q c_{qi} c_{qj} f_q^{(neq)}$$

A compiler  
can't do that!



```
Pxx =  n01 +n02 +n03 +n04 +n05 +n10 +n11 +n12 +n13 +n14
Pyy =  n01 +n03 +n07 +n08 +n09 +n10 +n12 +n16 +n17 +n18
Pzz =  n02 +n04 +n06 +n07 +n09 +n11 +n13 +n15 +n16 +n18
!
Pxz = -n02 +n04 +n11 -n13
Pxy = -n01 +n03 +n10 -n12
Pyz = +n07 -n09 +n16 -n18
...
```

Drastic operation reduction!

- ✓ **Only 36 sums**
- ✓ No multiplication at all
- ✓ no load of **cx (pop)** , **cy (pop)** , **cz (pop)** vectors



## other performance figures

- ✓ Left: time for  $256^3$  simulation with Smagorinsky Model (no optimized)
- ✓ Right: time for  $256^3$  simulation with Smagorinsky Model (optimized)

# Time for section			
# init	time	0.111767E+01	
# loop	time	0.866046E+02	
# coll	time	0.791241E+02	
# bc	time	0.645086E+01	
# diagno	time	0.101066E+01	

# Time for section			
# init	time	0.112207E+01	
# loop	time	0.730055E+02	
# coll	time	0.655008E+02	
# bc	time	0.646228E+01	
# diagno	time	0.102758E+01	

- ✓ Now the Smagorinsky impact is negligible...

---

## Comment (personal)

- ✓ Compilers can help you, but you must be aware of what they can or cannot do
  - ✓ Coding style can help/confuse compilers
  - ✓ Optimization capability of today compilers is decreasing
    - more optimization work is demanded to developers
  - ✓ Play with different compilers (if possible)
  - ✓ Play with different optimization level/flag
  - ✓ Use flags to understand what's going on under the hood
    - e.g. `-Minfo` for nvidia compilers
-

---

## Finite precision

A computer uses finite precision. This means that some rules are different respect infinite precision (standard algebra)

- ✓ **Sum is no more additive.** You can choose three number  $a, b, c$  so that

$$(a + b) + c \neq a + (b + c)$$

- ✓ in finite precision we have “many numbers” that behaves like a zero

$$(a + c) = a \rightarrow c \equiv 0$$

---

---

# Floating point: IEEE p754

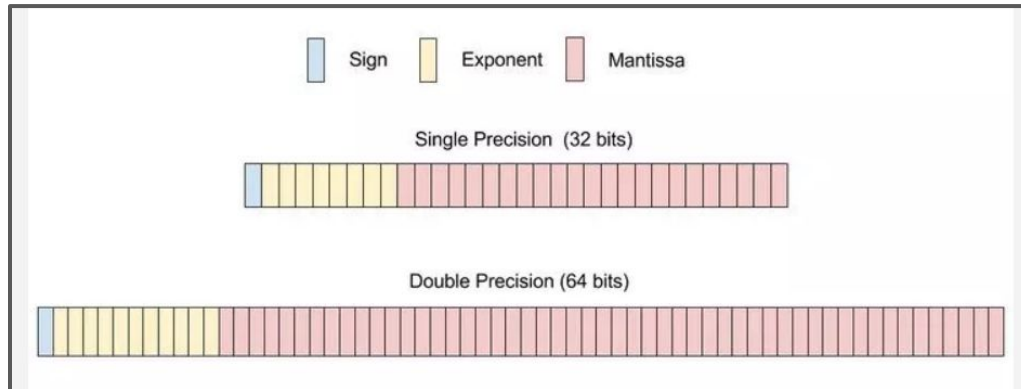
The **IEEE Standard for Floating-Point Arithmetic (IEEE 754)** is a technical standard for floating-point arithmetic established in 1985 by the Institute of Electrical and Electronics Engineers (IEEE). The standard addressed many problems found in the diverse floating-point implementations that made them difficult to use reliably and portably. Many hardware floating-point units use the IEEE 754 standard.

- ✓ ***arithmetic formats***: sets of binary and decimal floating-point data, which consist of finite numbers (including signed zeros and subnormal numbers), infinities, and special "not a number" values (NaNs)
  - ✓ ***interchange formats***: encodings (bit strings) that may be used to exchange floating-point data in an efficient and compact form
  - ✓ ***rounding rules***: properties to be satisfied when rounding numbers during arithmetic and conversions
  - ✓ ***operations***: arithmetic and other operations (such as trigonometric functions) on arithmetic formats
  - ✓ ***exception handling***: indications of exceptional conditions (such as division by zero, overflow, etc.)
-

# Floating point: binary representation

- ✓ Machine Epsilon: minimum non zero value with respect to 1.0
- ✓ Range: max/min values that can be represented

Precisione	Precisione $p$	Machine epsilon	Range
Singola	24	$2^{-23} \simeq 1.2 \times 10^{-7}$	$10^{-38} < x < 10^{38}$
Doppia	53	$2^{-52} \simeq 1.2 \times 10^{-16}$	$10^{-308} < x < 10^{308}$



## Cancellation issue

- ✓ Cancellation happens when we have big and little number to add/subtract
- ✓ Programmer has to take care (with parentheses) of the right order to save “bits”
- ✓ **But compiler can alter the order and produce wrong results**
- ✓ for  $a = 0.333333$  we perform different operation with different values of  $b$  (single precision)

	$b = 1.60$	$b = 6553.6$	$b = 3355443$	$b = 1.3421773E+07$
$b - b + a$	0.3333333	0.3333333	0.3333333	0.3333333
$b + a - b$	0.3333334	0.3334961	0.2500000	0.0000000E+00
$a + b - b$	0.3333334	0.3334961	0.2500000	0.0000000E+00
$a - b + b$	0.3333334	0.3334961	0.2500000	0.0000000E+00

- ✓ **Solution:** “Group” quantities with the same numerical range

---

# Single vs. Double precision

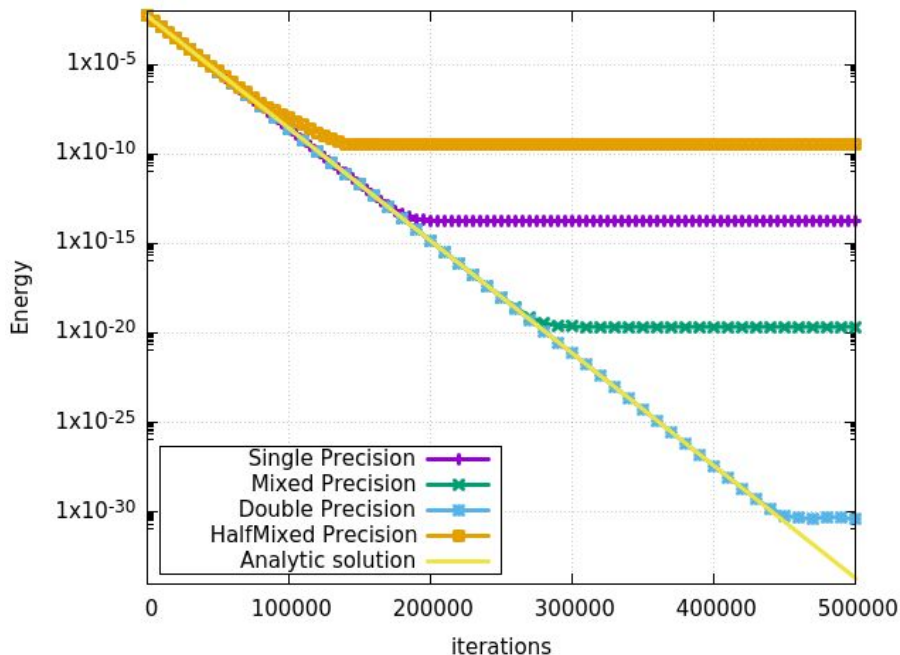
- ✓ Double precision has a wider range respect single precision and is less subject to cancellation issues
- ✓ But today **HW is two times faster** (or even more) for single precision computation respect double one (do you remember vectorization?)
  - Now it happens for both CPU and GPU
- ✓ **Half precision is 4 times faster** respect double precision
  - GPU and next generation CPU (it is used for ML)

## Hint:

- ✓ Check if single precision is fine for you and you problem
  - ✓ Use mixed precision: i.e., single precision for stored data, double for all computation
  - ✓ Use compiler flags to check if you code is IEEE compliant
-

# TG-Vortex:example

- ✓ Taylor-Green Vortices are a 2D flow configuration where energy decay has an analytical exponential law.
- ✓ Performance (right) in MLUPs, higher is better (GPU)



Precision	MLUPs
Half/Single-	11844
Single	7296
Single/Double	7314
Double/Double	4369



# HW trends/1

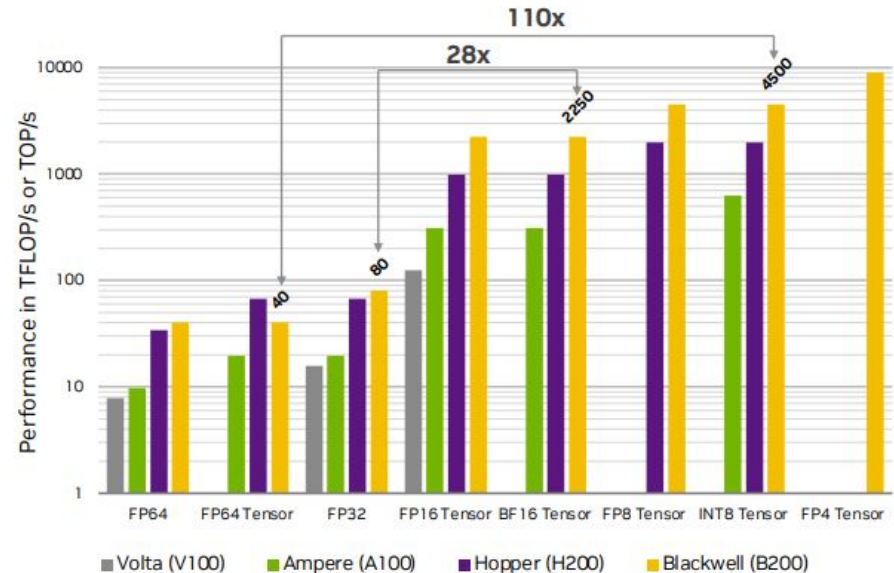
- ✓ GPU are today the building block of HPC cluster
- ✓ HW is developed not according to HPC needs
- ✓ “mala tempora currunt”
- ✓ NVIDIA GPUs evolution

Figure of Merit	Volta 2017 (V100)	Ampere 2020 (A100)	Hopper 2022 (H200)	Blackwell 2024 (B200)
FP64 FMA (TFLOP/s)	7.8	9.75	33.5	40
FP64 Tensor (TFLOP/s)	N/A	19.5	67	40
FP32 FMA (TFLOP/s)	15.7	19.5	67	80
FP16 Tensor (TFLOP/s)	125	312	989	2250
BF16 Tensor (TFLOP/s)	125	312	989	2250
INT8 Tensor (TOP/s)	N/A	624	1979	4500
Memory BW (TB/s)	0.9	2.0	4.8	8.0

## HW trends/2

It is possible to obtain double precision resolution using lower precision:

- ✓ DGEMM on Integer Matrix Multiplication Unit
- ✓ Boosting Matrix Multiplication Speed and Flexibility with NVIDIA cuBLAS 12.9



# Finite precision issues: computing Pi

- ✓ Simple way to compute Pi

$$\frac{\pi^2}{6} = \sum_{n=1}^{\infty} \frac{1}{n^2}$$

```
! forward sum...
  do i=1,elements
    sum1=sum1+(1.0/(float(i)*float(i)))
  end do

!
! backward sum
  do i=elements, 1, -1
    sum2=sum2+(1.0/(float(i)*float(i)))
  end do

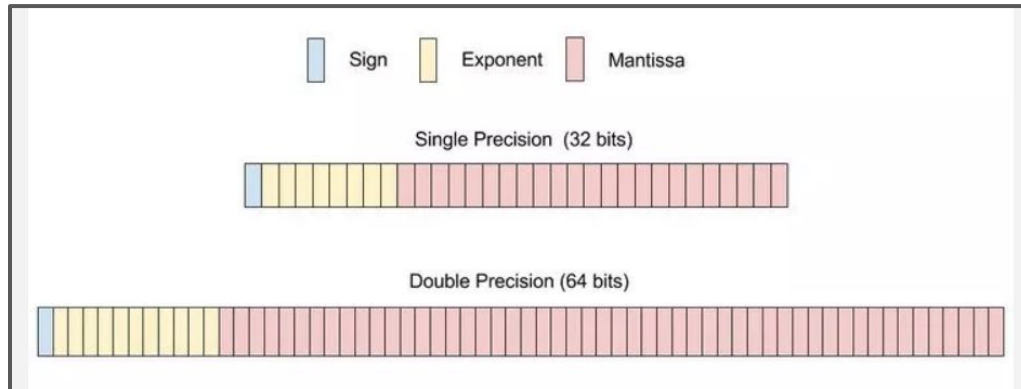
...

write(6,*) 'forward =', sqrt(6.0*sum1)
write(6,*) 'backward=', sqrt(6.0*sum2)
```

# Recap: Floating point binary representation

- ✓ Machine Epsilon: minimum non zero value with respect to 1.0
- ✓ Range: max/min values that can be represented

Precisione	Precisione $p$	Machine epsilon	Range
Singola	24	$2^{-23} \simeq 1.2 \times 10^{-7}$	$10^{-38} < x < 10^{38}$
Doppia	53	$2^{-52} \simeq 1.2 \times 10^{-16}$	$10^{-308} < x < 10^{308}$



# Finite precision issues: computing PI

- ✓ The Backward sum is more precise with respect to Forward sum
- ✓ Why?

Elements	Ratio (Backward)	Ration (Forward)
100	0.9969709148	0.9969709907
1'000	0.9996961603	0.9996962361
10'000	0.9999695955	0.9999365829
100'000	0.9999969162	0.9999365829
1'000'000	0.9999997242	0.9999365829
10'000'000	0.9999999519	0.9999365829

---

## I/O issues

- ✓ I/O operations are really expensive
  - Cycles are order of nanoseconds
  - Memory access are order of 100 or 1000 cycles
  - I/O access can be order of 100000 cycles (milliseconds)
- ✓ Writing on rotating disks implies great latencies

### Golden rules

**#1: write/read on the disk only if it is mandatory**

**#2: write/read only what is really important**

**#3: always use binary and never formatted data (e.g. ASCII) for “huge” dump**

---

# I/O Example

✓ I/O operations are really expensive

```
! formatted
do k=1,nd
  do j=1,nd
    do i=1,nd
      write(69,*) a(i,j,k)
    enddo
  enddo
enddo
```

```
! unformatted (1)
do k=1,nd
  do j=1,nd
    do i=1,nd
      write(79) a(i,j,k)
    enddo
  enddo
enddo
```

```
! unformatted (2)
write(82)
((a(i,j,k),i=1,nd),j=1,nd),k=1,nd)
```

```
! unformatted (3)
write(83) a
```

---

# I/O Example

- ✓ I/O operations are really expensive
- ✓ Time writing on /scratch
- ✓ Time presented here only as relative reference (old stuff)
  - It heavily depends from the filesystem configuration

	time (sec.)
<b>Formatted</b>	6.88
<b>unformatted-1</b>	1.41
<b>unformatted-2</b>	0.34
<b>unformatted-3</b>	0.10



---

# I/O Some strategies

- ✓ I/O is the bottleneck: avoid it when possible
- ✓ I/O subsystem work with locks: simplify application
- ✓ I/O has its own parallelism: use MPI-I/O or other libraries
- ✓ I/O is slow: compress (to reduce) output data
- ✓ Raw data could be not portable: use library
- ✓ I/O C/Fortran APIs are synchronous: use dedicated I/O tasks
- ✓ Application DATA are too large: analyze it “on the fly”, (e.g. re-compute vs. write)

**Carefully plan your data production/workflow BEFORE the simulation**

# Moving Data

Bits per Second Requirements

<b>10PB</b>	25,020.0 Gbps	3,127.5 Gbps	1,042.5 Gbps	148.9 Gbps	34.7 Gbps
<b>1PB</b>	2,502.0 Gbps	312.7 Gbps	104.2 Gbps	14.9 Gbps	3.5 Gbps
<b>100TB</b>	244.3 Gbps	30.5 Gbps	10.2 Gbps	1.5 Gbps	339.4 Mbps
<b>10TB</b>	24.4 Gbps	3.1 Gbps	1.0 Gbps	145.4 Mbps	33.9 Mbps
<b>1TB</b>	2.4 Gbps	305.4 Mbps	101.8 Mbps	14.5 Mbps	3.4 Mbps
<b>100GB</b>	238.6 Mbps	29.8 Mbps	9.9 Mbps	1.4 Mbps	331.4 Kbps
<b>10GB</b>	23.9 Mbps	3.0 Mbps	994.2 Kbps	142.0 Kbps	33.1 Kbps
<b>1GB</b>	2.4 Mbps	298.3 Kbps	99.4 Kbps	14.2 Kbps	3.3 Kbps
<b>100MB</b>	233.0 Kbps	29.1 Kbps	9.7 Kbps	1.4 Kbps	0.3 Kbps
	<b>1H</b>	<b>8H</b>	<b>24H</b>	<b>7Days</b>	<b>30Days</b>

---

## Recap

- ✓ i/O is very slow
  - ✓ I/O is very very slow
  - ✓ I/O is very very very slow
  - ✓ Have I pointed out that I/O is slow already?
  - ✓ the compiler is your best friend, but sometimes your worst enemy
  - ✓ take care of floating point operation
  - ✓ Code refactoring is crucial: a “clean” code is important, but could be inefficient
-

---

## References

- ✓ [D. Goldberg. 'What every computer scientist should know about floating-point arithmetic'. Computing Survey of ACM, March 1991.](#)
  - ✓ [M. L Overton. 'Numerical computations with IEEE Floating Point Arithmetic'. SIAM, 2001.](#)
  - ✓ M. Abramowitz and I. Stegun. 'Handbook of Mathematical Functions' 1974
  - ✓ [J.H. Wilkinson. 'Rounding errors in algebraic processes'. Dover.](#)
  - ✓ Dongarra et al. ['Investigating half precision arithmetic to accelerate dense linear system solvers'](#)
-