Introduction into Hardware and parallel concepts

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What do you have to expect?

Tutorial with practical work

I) Parallel concepts; Hardware; Relations inbetween; The example environment

II) PDE; Finite Element discretization; System of equations; (simple) iterative solver; parallelization concept

III) Classical shared memory and distributed parallelization parallelization (OpenMP and MPI)

IV) Accelerator programming for NVIDIA GPU; practical work (OpenACC and CUDA)

V) Distributed computing with multiple GPUs; practical work

Parallel concepts

Classification by memory access

- Distributed memory access
  - cluster computing; multi-core computing
  - MPI (Message Passing Interface)
- Shared memory access
  - multi-core computing, many-core computing
  - OpenXXX, CUDA, OpenCL
  - distributed shared memory on compute clusters available.
- Faked shared memory access
  - distributed shared memory on compute clusters available (hardware!!).
  - PGAS (partitioned global address space)

UMA: uniform memory access
NUMA: non-uniform memory access
ccNUMA: cache coherent NUMA
hUMA: heterogeneous UMA (by AMD)

bandwidth: byte per second in a data transfer from/to memory ($\mathcal{O}(\frac{1}{t_{\text{bandwidth}}})$)
latency: time until data transfer starts t_{latency}
Transferring n Byte: $t(n) = t_{\text{latency}} + n * t_{\text{bandwidth}}$

Memory hierarchies

- Normal DRAM (Dynamic Random Access Memory) stores a bit in a capacitor
  - needs only a few transistors $\Longrightarrow$ small area on chip, cheap
  - large amount of memory
  - needs refreshment cycles $\Longrightarrow$ slow access
- Cache SRAM (Static Random Access Memory) stores a bit in a flip-flop circuit
  - needs more transistors $\Longrightarrow$ larger area on chip, expensive
  - small amount of memory
  - no refreshment cycles $\Longrightarrow$ fast access
- Therefore, DRAM is combined with a hierarchy of smaller but faster caches.

Non **U**niform **M**emory **A**ccess (wrt. latency and bandwidth)

- CPU:
  Register – L1 – L2 – L3-cache – memory – remote memory
- GPU:
  Register – shared/L1 – L2 – GPU memory – CPU memory

Classification by streams [Flynn, 1966]

Data stream vs. Instruction stream

Instruction Stream			
Single	Multiple		
SISD	**MISD**	Single	Data
SIMD	**MIMD**	Multiple	Stream

Table: Flynn's taxonomy

SISD (Single Instruction Single Data) is the classical sequential von-Neumann computer.

MISD (Multiple Instruction Single Data) can be found in the pipelining of instruction in modern processors and in flight control computers.

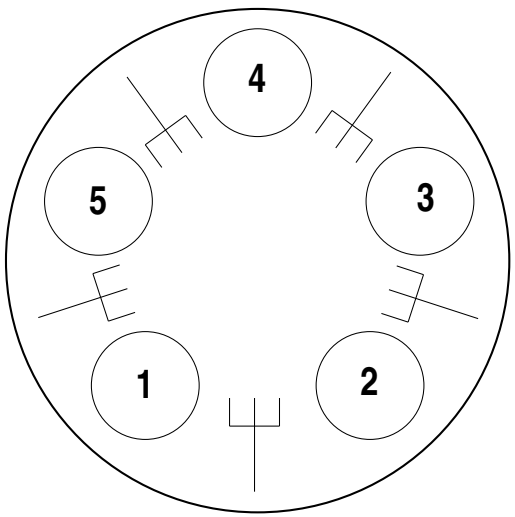
Our focus will be on **MIMD** and **SIMD**.

MIMD - Multiple Instructions Multiple Data

- Each process (and its instructions) access data on different ressources (i.e., distributed memory)
- Often as SPMD (Single Programm Multiple Data)
- explicit access to ressources of other processes via communication.
- $\Longrightarrow$ dead locks might block the whole code
- MPI (Message Passing Interface)

Dead lock: Dinner for five [Dijkstras 1971]

Dead lock: *Processes have to wait for an event that has to be performed by one of the waiting processs.*



5 philosophers (P) with 5 forks (R).
Each P needs two forks (R) for eating:

1. Each philospher takes the the right fork and waits for the left fork. $\Longrightarrow$ Dead lock for all (starving with one fork in their hand)
2. Wait until both forks are available, eat and release them afterwards $\Longrightarrow$ Dead lock for one (P_1, P_3) eat alternating with (P_5, P_2) and P_4 starves

A dead lock for all is obvious but a dead lock for one might be very subtle to find.

SIMD - Single Instruction Multiple Data

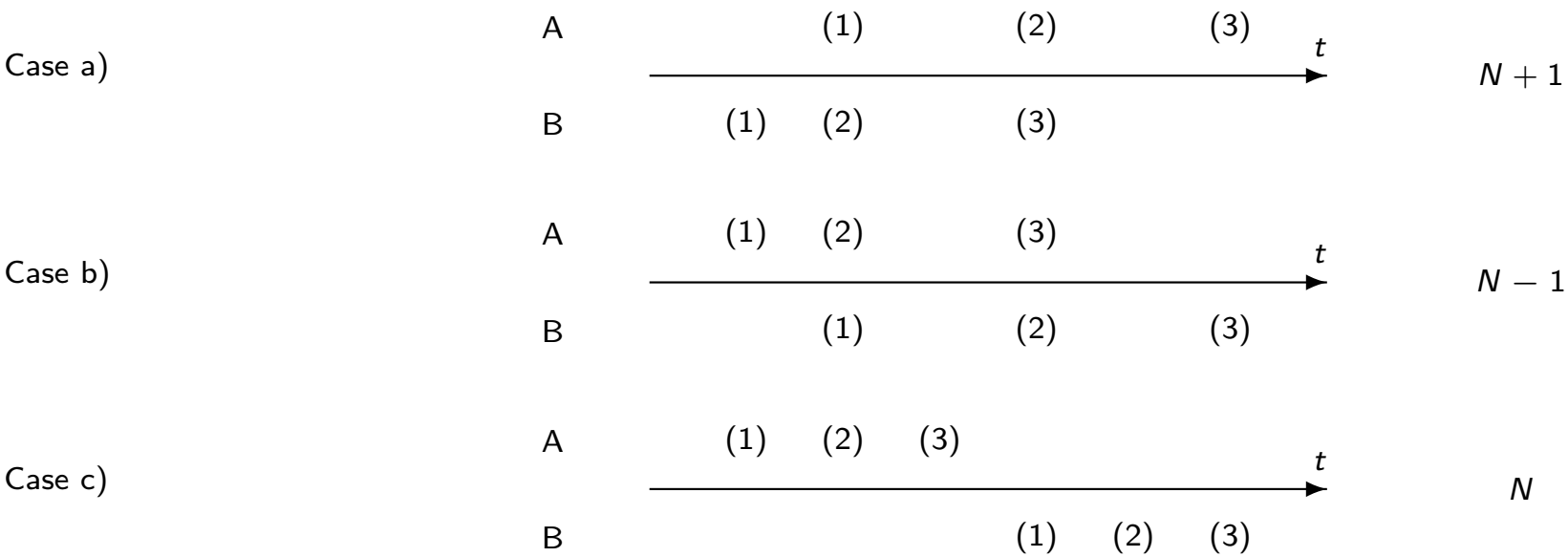
- Each thread (and its instructions) accesses data on shared ressources (e.g., shared memory)
- implicit access to ressources of other threads.
- $\Longrightarrow$ data races result in unpredictable (incorrect) results
- OpenXXX, CUDA, OpenCL
- A SIMT (Single Instruction Multiple Threads) per warp on GPUs available.
  - 1 instruction pointer per b threads in one warp
  - all b threads have to wait for slowest thread (alternatives, while-loops)

Data Race

Uncoordinated manipulation of shared ressources.

thread A: $N := N + 1$	clock.	thread B: $N := N - 1$
`load` N	(1)	`load` N
`inc` N	(2)	`dec` N
`store` N	(3)	`store` N

The value of N is not predictable, it depends on the execution speed of threads A and B

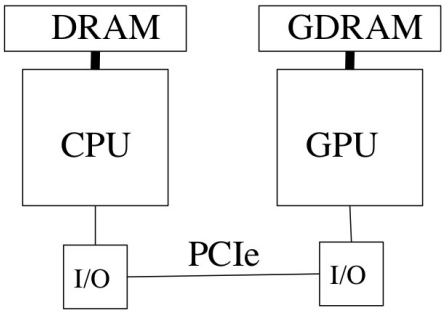


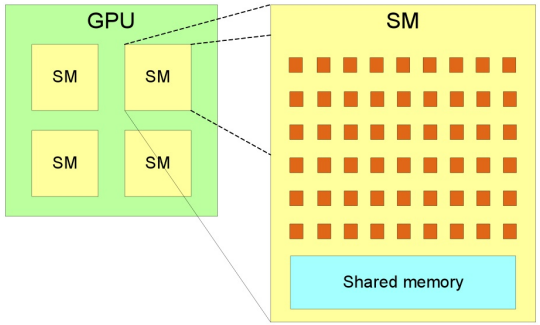
Data race: solution

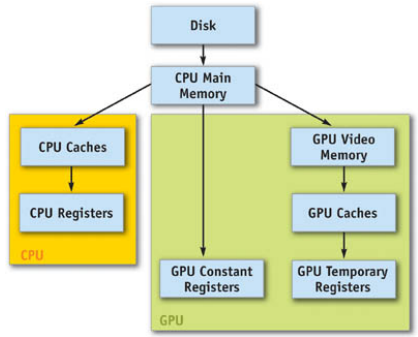
- Consider the operations `load`, `inc`/`dec`, `store` as **one atomic** operation.
- This atomic operation has to be finished before another thread gets access to the ressources.
- $\Longrightarrow$ N will be locked.
- N in local cache requires ccNUMA (Hey, that value has been changed!).

- For-loops for vector operation $\underline{z} = \alpha \cdot \underline{z} + \underline{y}$ followed by $\underline{a} = \underline{z} + \underline{b}$ might require thread synchronization between loops.
  (`#pragma omp barrier`)

What is new in accelerator programming?







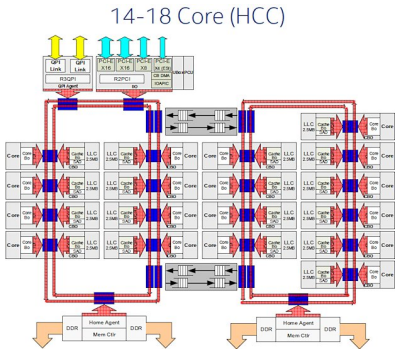
©PRACE
©NVIDIA

- 2 levels of shared memory on GPU: global for GPU + local on SM
- **Host**: Usually a CPU core
- **Device**: Accelerator device as GPU or Xeon Phi (or multi-core CPU)
- seperate memory with explicit data transfer between host and device memory
- memory(host) >> memory(device)
- bandwidth(host)< bandwidth(device)
- Synchronization between threads only locally on SM, not globally.
- Threads in one warp are parallel by instruction (one IP for all)

Hardware remarks

Processor types on the market (2014)

CPU
Xeon E7-8890 v2



18 cores, 1.5TB
108 GByte/sec
≈750 GFLOPS(d,peak)
AVX2 (512)
145 Watt

SIMT/SIMD (MIMD)
g++, OpenMP

Cluster on DIE;

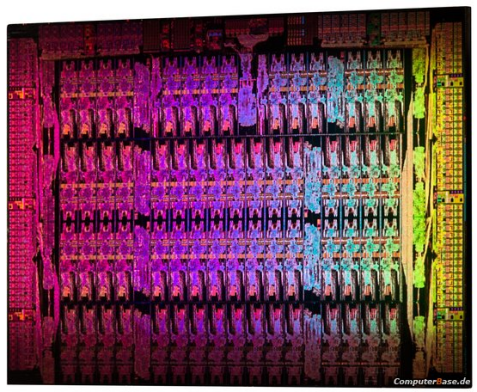
GPU
Tesla K40

15 × 192 cores, 12 GB
288 GByte/sec
1.4 TFLOPS (d,peak)
235 Watt

SIMT + MIMD
CUDA, OpenACC

incl. GPUs + OpenACC;

MIC
Xeon Phi 7120P



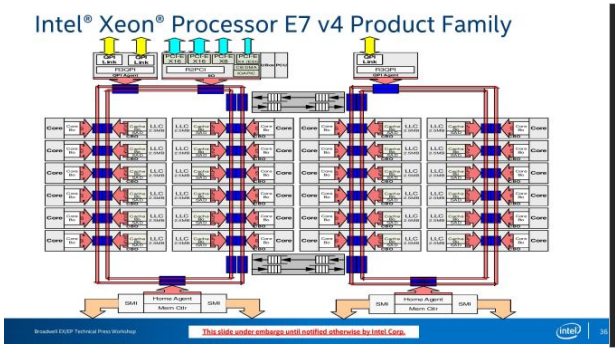
61 cores, 16 GB
352 GByte/sec
1.2 TFLOPS (d,peak)
AVX (512)
300 Watt

SIMT/SIMD (MIMD)
Intel-Compiler,
OpenMP 4.0

MIC (Many Integrated Core);

Processor types on the market (2017)

CPU
Xeon E7-8890 v4

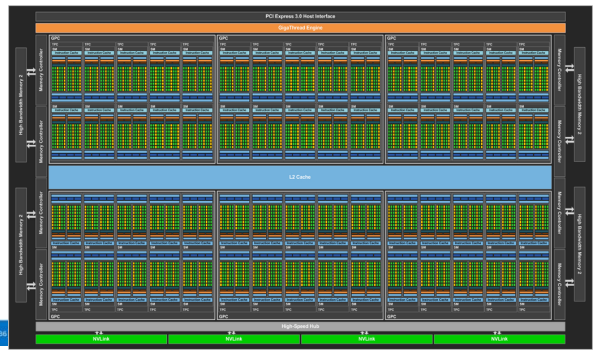


24 cores, 1.5TB
85 GByte/sec
≈844 GFLOPS(d,peak)
AVX2 (512)
165 Watt

SIMT/SIMD (MIMD)
g++, OpenMP

Cluster on DIE;

GPU
Tesla P100



56 × 64 cores, 16 GB
732 GByte/sec
4.7 TFLOPS (d,peak)
300 Watt

SIMT + MIMD
CUDA, OpenACC

incl. GPUs + OpenACC;

KNL
Xeon Phi 7290F

72 cores, 16 GB
400+ GByte/sec
3.45 TFLOPS (d,peak)
AVX512
260 Watt

SIMT/SIMD (MIMD)
Intel/GNU, OpenMP

MIC (Many Integrated Core);

Programming Models in multi-/many-core environments

- distributed memory: MPI ⊥

- vectorization: SSE, AVX ⟶ compiler support (`#pragma omp simd`)
- shared memory: OpenMP ⟶ compiler support (`#pragma omp parallel for`)
- many-core:
  - GPU-systems: CUDA, OpenCL, OpenACC (⟶ general devices)
  - general: OpenACC (`#pragma acc parallel loop`)
    commercial compiler support since spring 2012
    [Nov 13, 2011; Cray, Nvidia, PGI]
  - MIC-systems: OpenMP 4.0 (⟶ general devices) (`#pragma omp target`)
    [July 2013: AMD, Cray, Intel, IBM, NVIDIA, ...]

Shared memory: first example

seq: Scalar product

$$s = \langle x, y \rangle = \sum_{k=0}^{N-1} x_k \cdot y_k$$

Listing 1: Scalar product

```
double scalar(int N, const double x[], const double y[])
{
    double sum = 0.0;
    for (int i=0; i<N; ++i)
    {
        sum += x[i]*y[i];
    }
    return sum;
}
```

dualhex: 2× AMD Opteron 2427, 6x 2.20GHz, 32 GB

N=250 Mill., 50 outer loops

1 core: **0.78 sec.**

shm: Scalar product – race condition

Listing 2: Scalar product with race condition

```
double scalar(int N, const double x[], const double y[])
{
    double sum = 0.0;
    int i;
#pragma omp parallel for private(i) shared(x,y,sum)
    for (i=0; i<N; ++i)
    {
        sum += x[i]*y[i];
    }
    return sum;
}
```

dualhex:
N=250 Mill., 50 outer loops

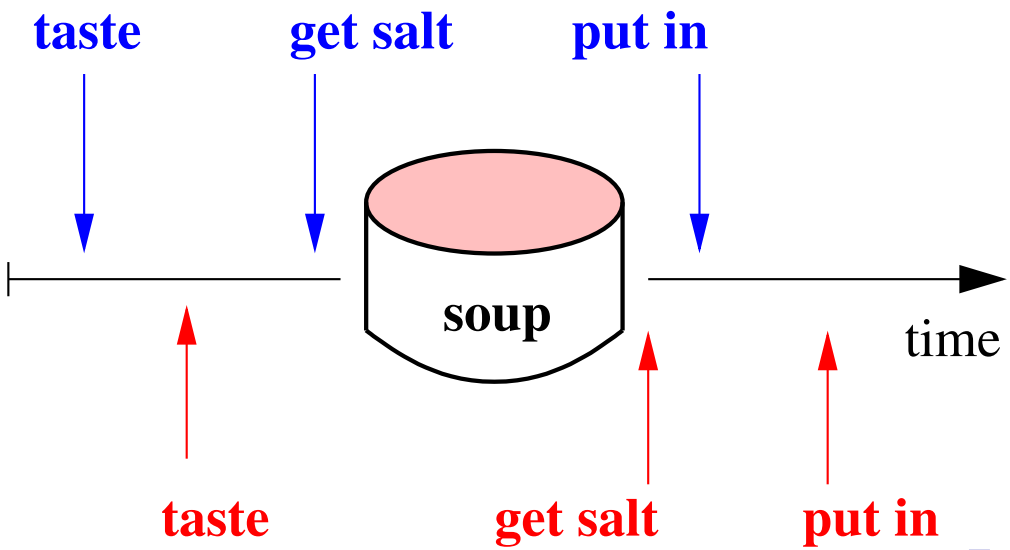
4 cores: **0.81 sec.**

Easy, but wrong result because of data race.

shm: data race – two cooks

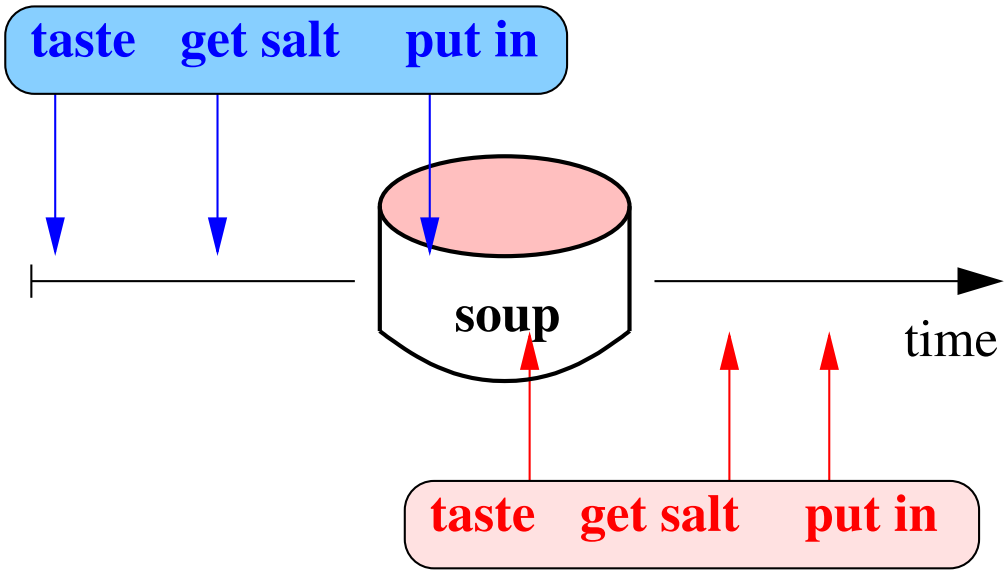
Listing 3: Scalar product with data race

```
double scalar(int N, const double x[], const double y[])
{
    double sum = 0.0;
    int i;
#pragma omp parallel for private(i) shared(x,y,sum)
    for (i=0; i<N; ++i)
    {
        sum += x[i]*y[i];
    }
    return sum;
}
```

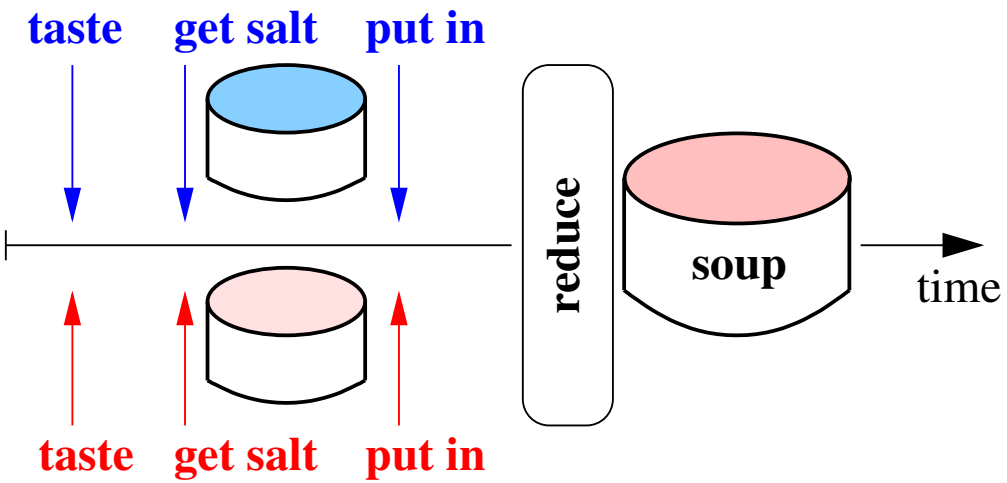


shm: two cooks – atomic vs. reduce

atomic:



reduce:



shm: Scalar product – atomic

Listing 4: Scalar product with atomic pragma

```
double scalar(int N, const double x[], const double y[])
{
    double sum = 0.0;
#pragma omp parallel for shared(x,y,sum)
    for (int i=0; i<N; ++i)
    {
#pragma omp atomic
        sum += x[i]*y[i];
    }
    return sum;
}
```

dualhex:
N=250 Mill., 50 outer loops 4 cores: **38 sec.**

correct result but slow because of atomic operation.

shm: Scalar product – reduce

Listing 5: Scalar product with reduction

```
double scalar(int N, const double x[], const double y[])
{
   double sum = 0.0;
#pragma omp parallel for shared(x,y) reduction(+:sum)
   for (int i=0; i<N; ++i)
   {
      sum += x[i]*y[i];
   }
   return sum;
}
```

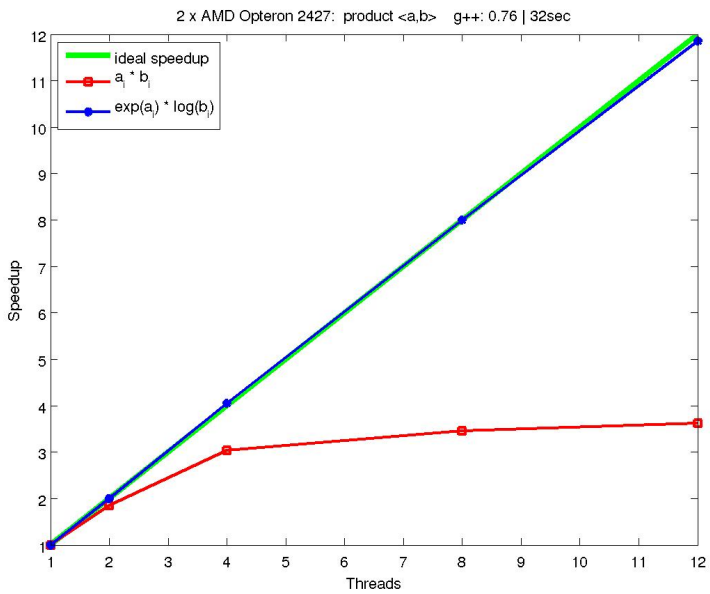
dualhex:
N=250 Mill., 50 outer loops

4 cores: **0.48 sec.**
(1 core: 0.78 sec.)

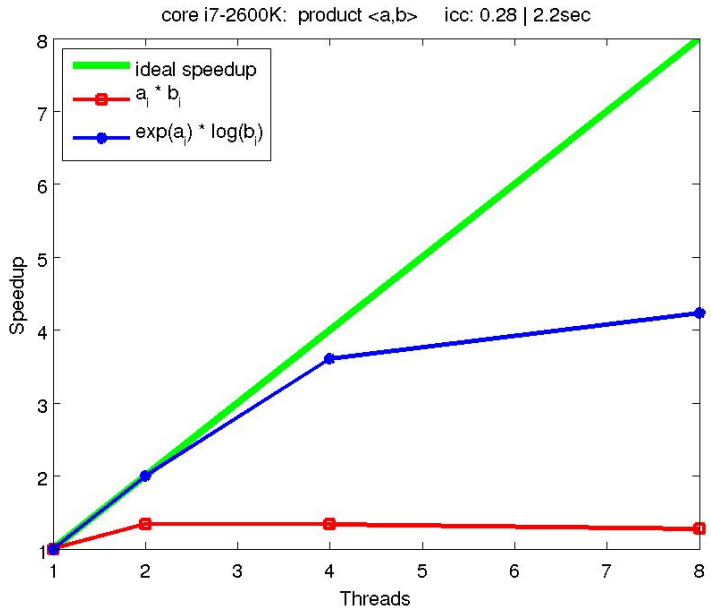
Easy, correct result.

Shared Memory: speedup

12-core Opteron



4-core SandyBridge



* poor speedup for $\sum_{k=0}^{N-1} x_k \cdot y_k$:

limited by memory bandwidth

* excellent speedup for $\sum_{k=0}^{N-1} \exp(x_k) \cdot log(y_k)$:

limited by functional units

Shared memory: non-Newtonian fluid

Diego A. Vasco
[Universidad de Santiago de Chile]

Mathematical Modeling

- Laminar
- Incompressible
- Non Newtonian

$$\nabla \cdot \vec{v} = 0$$

Continuity equation

Non Newtonian

$$\frac{\partial}{\partial t}\rho\vec{v} + \left(\vec{v}\cdot\nabla\right)\rho v = -\nabla p + \nabla\cdot\tau + \rho\cdot\vec{b}$$

Navier –Stokes Equation

$$\rho Cp\left(1 + \frac{h_{ls}}{\rho Cp}\frac{\partial f_{pc}}{\partial T}\right)\left[\frac{\partial T}{\partial t} + \left(\vec{v}\cdot\nabla\right)T\right] = -\left(\nabla\cdot q\right) + \tau : D$$

Conservation of Energy

Phase Change

Viscous Disipation

$$\frac{\partial F}{\partial t} + \vec{v}\cdot\nabla F = 0$$

Free Boundary (VOF)

Mathematical Modeling

Constitutive Equations

Shear stress tensor

$$\tau = \begin{vmatrix} \tau_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \tau_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \tau_{zz} \end{vmatrix}$$

Normal components

$$\tau_{xx} = -\eta\left[2\frac{\partial u}{\partial x}\right]$$

$$\tau_{yy} = -\eta\left[2\frac{\partial v}{\partial y}\right]$$

$$\tau_{zz} = -\eta\left[2\frac{\partial w}{\partial z}\right]$$

Tangencial components

$$\tau_{yz} = \tau_{zy} = -\eta\left[\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}\right]$$

$$\tau_{xy} = \tau_{yx} = -\eta\left[\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right]$$

$$\tau_{xz} = \tau_{zx} = -\eta\left[\frac{\partial w}{\partial x} + \frac{\partial u}{\partial z}\right]$$

Shear rate tensor

$$\Delta_{ij} = \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}$$

$$I_1 = (\Delta : \delta) \qquad I_2 = (\Delta : \Delta) \qquad I_3 = det\,\Delta$$

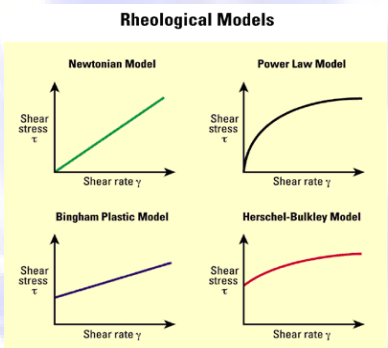
Mathematical Modeling

$$\dot{\gamma} = \sqrt{\frac{1}{2}(\Delta : \Delta)}$$

Generalized Newtonian Models

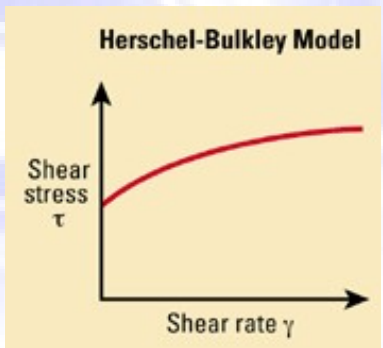
Power Law

$$\eta = k\,\dot{\gamma}^{n-1}$$



Herschel-Bulkley

$$\eta = \frac{\tau_0}{\dot{\gamma}} + k\,\dot{\gamma}^{n-1}$$



Carreau-Yasuda

$$\eta = \eta_\infty + (\eta_0 - \eta_\infty) + \left(1 + \left(k\,\dot{\gamma}\right)^a\right)^{n-1/a}$$

Cross

$$\eta = \eta_\infty + \frac{\eta_0 - \eta_\infty}{1 + \left(k\,\dot{\gamma}\right)^m}$$

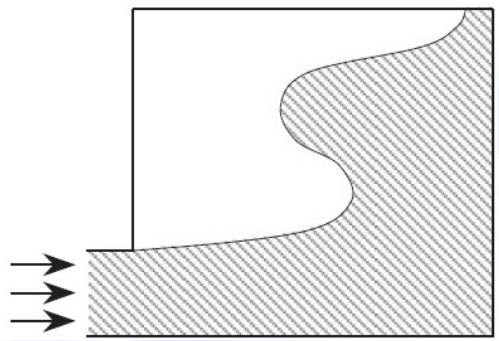
Mathematical Modelin

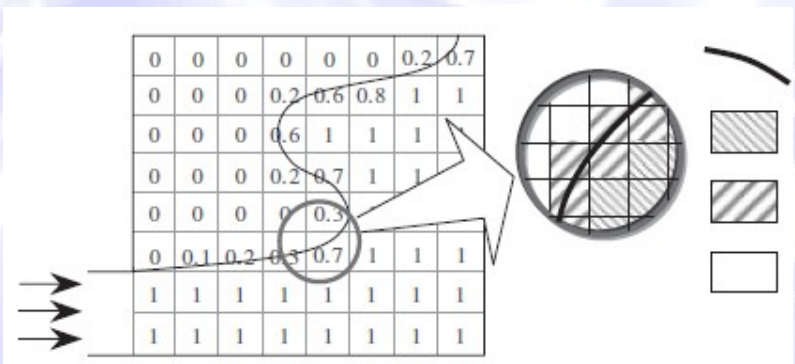
Moving Boundary

VOF (Volume of Fluid) Method

$$\frac{\partial F}{\partial t} + \vec{v} \cdot \nabla F = 0$$

$$\int_V \frac{\partial F}{\partial t} dV + \int_s F \, \vec{v} \cdot \hat{n} \, ds = 0$$





Position of the interphase

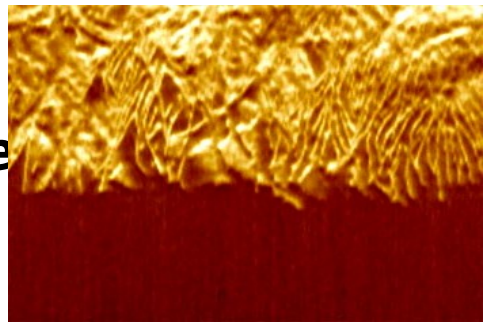
Full	$F = 1$
Partially full	$0 < F < 1$
Empty	$F = 0$

M. Kim, W. Lee International Journal for Numerical Methods in Fluids 42 (2003) 765-790.

Mathematical Modeling

Phase Change

- **Defined**: Pure Metals
- **Alloy**: Complex interphase
- **Continuos**: Polymers



$$\frac{\partial H}{\partial t} = \nabla \cdot \left(k \nabla T \right)$$

$$f_{pc} \approx f_{pc}(T)$$

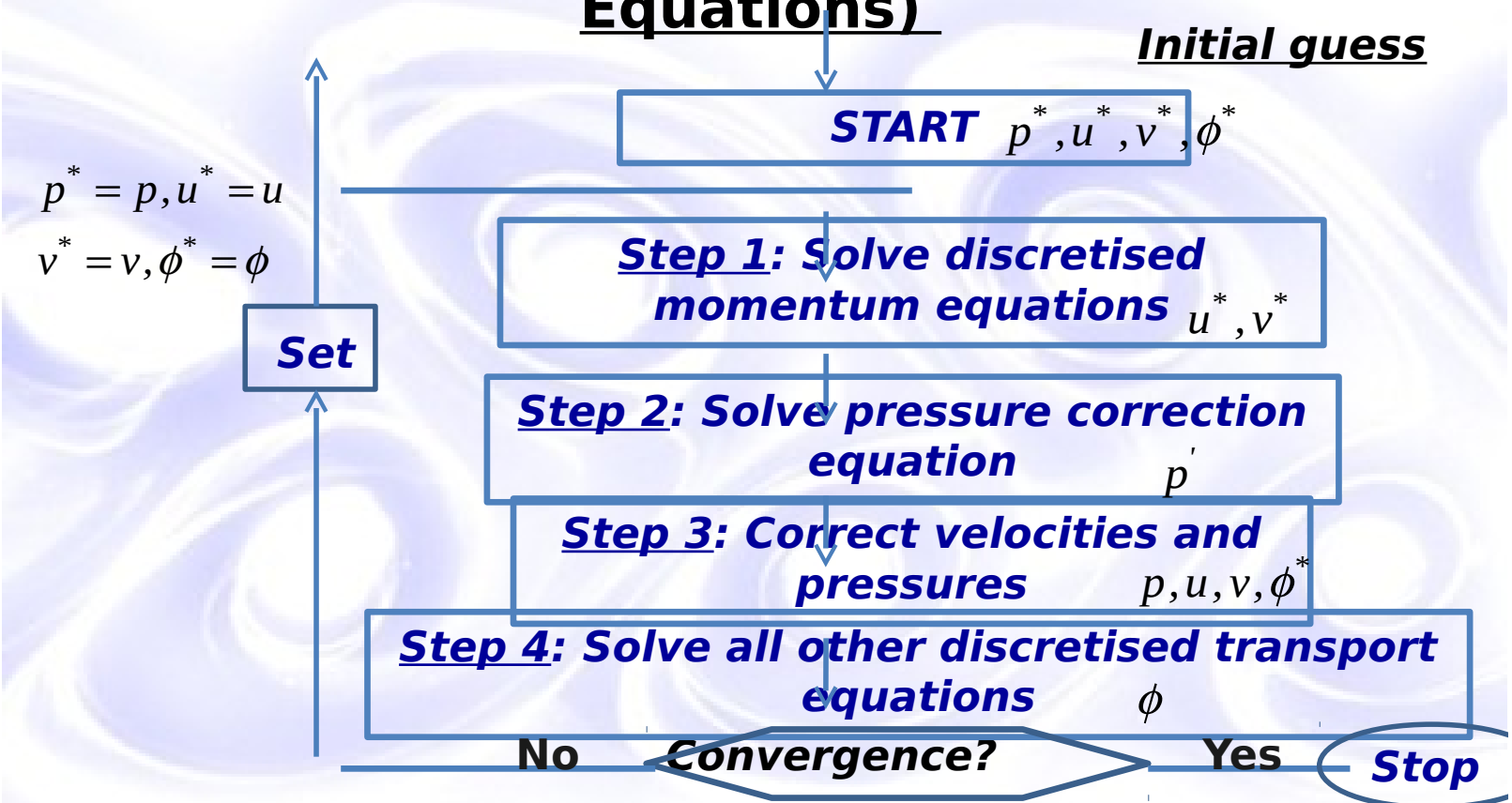
$$f_{PC} = \begin{cases} 0 & T \le T_s \\ \left(\dfrac{T - T_s}{T_l - T_s} \right)^m & T_s < T < T_l \\ 1 & T \ge T_l \end{cases}$$

$$\rho Cp \left(1 + \frac{h_{ls}}{\rho Cp} \frac{\partial f_{pc}}{\partial T} \right) \frac{\partial T}{\partial t} = \nabla \cdot \left(k \nabla T \right)$$

C. Beckermann, Melting and solidification of binary systems with double-diffusive convection in the melt, Ph.D Thesis, Purdue University (1987)

SIMPLE

(Semi-Implicit Pressure Linked Equations)



Versteeg & Malalasekera, An Introduction to computational fluid dynamics, Longman, NY, (1995)

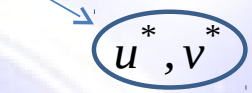
SIMPLE

(Semi-Implicit Pressure Linked Equations,_

Step 1

$$a_{i,j}u^*_{i,j} = \sum_{nb} a_{nb}u^*_{nb} + \left(P^*_{i-1,j} - P^*_{i,j}\right)A_{i,j} + b_{i,j}$$

$$a_{i,j}v^*_{i,j} = \sum_{nb} a_{nb}v^*_{nb} + \left(P^*_{i,j-1} - P^*_{i,j}\right)A_{i,j} + b_{i,j}$$



Step 2

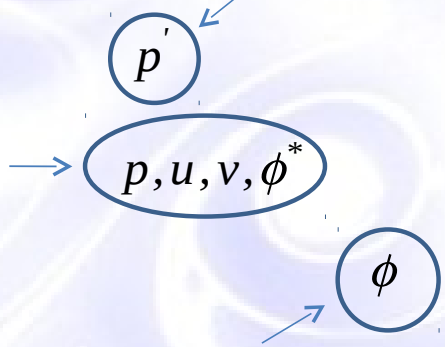
$$a_{i,j}p'_{i,j} = a_{i-1,j}p'_{i-1,j} + a_{i+1,j}p'_{i+1,j} + a_{i,j-1}p'_{i,j-1} + a_{i,j+1}p'_{i,j+1} + b'_{i,j}$$

Step 3

$$P_{i,j} = P^*_{i,j} + P'_{i,j}$$

$$u_{i,j} = u^*_{i,j} + d_{i,j}\left(P'_{i-1,j} - P'_{i,j}\right)$$

$$v_{i,j} = v^*_{i,j} + d_{i,j}\left(P'_{i,j-1} - P'_{i,j}\right)$$

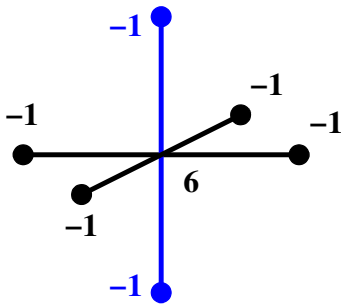


Step 4

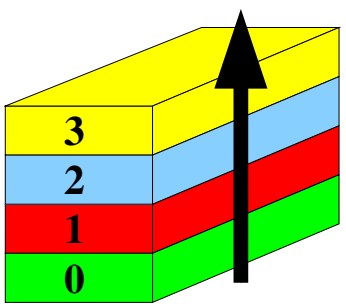
$$a_{i,j}\phi_{i,j} = a_{i-1,j}\phi_{i-1,j} + a_{i+1,j}\phi_{i+1,j} + a_{i,j-1}\phi_{i,j-1} + a_{i,j+1}\phi_{i,j+1} + b\phi_{i,j}$$

Solve linear system in each inner step

- system of coupled non-linear second order PDEs $\overset{\text{SIMPLE}}{\Longrightarrow}$ sequence of linear PDEs.
- unit cube, 7-point difference stencil



- Gauss-Seidel (forw/backw) wrt. plains in z-direction and
- ADI (Alternating Directions Iterative methods) in each plain
- shm parallel: combine plaines to a block Jacobi with above Gauss-Seidel in each block.



shm: system solve - naive approach

Listing 6: block-Jacobi Gauss-Seidel (shuffling)

```
...
  !$omp parallel do shared(app) schedule(static)
    do k = 1, N                    //  plain k: forward
       .....
       app(i,j,k)  = ....          //  cube data
    end do
                                   //

 !$omp parallel do shared(app) schedule(static)
    do k = N, 1, -1                //  plain k: backward
       .....
       app(i,j,k) += ....          //  cube data
    end do
...
```

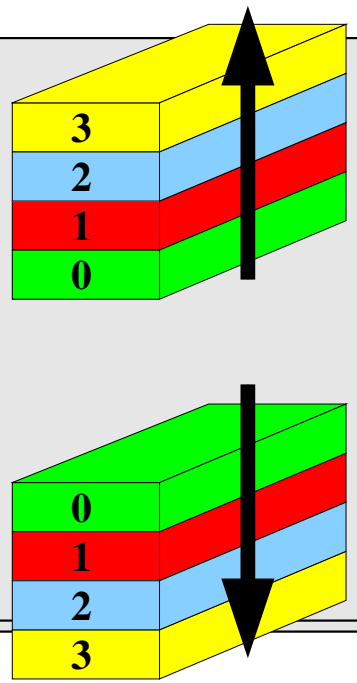
slower than on one thread

shm: system solve - naive approach

Listing 7: block-Jacobi Gauss-Seidel (shuffling)

```
...
  !$omp parallel do shared(app) schedule(static)
    do k = 1, N                          //  plain k
       .....
       app(i,j,k)  = ....                //  cube data
    end do
                                         //  data shuffling !!!!!!!

 !$omp parallel do shared(app) schedule(static)
    do k = N, 1, -1                      //  plain k
       .....
       app(i,j,k) += ....                //  cube data
    end do
...
```



slower than on one thread

$\Longleftarrow$ data blocks are remapped onto threads (data transfer!!)

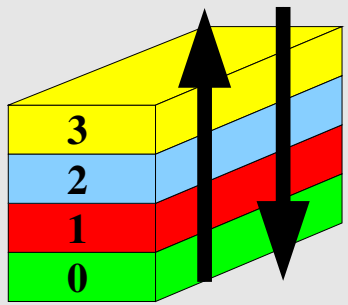
shm: system solve - better approach

Listing 8: block-Jacobi Gauss-Seidel (no shuffling)

```
...
  !$omp parallel shared(app) schedule(static)
  nthrd = omp_get_num_threads()          // number of threads
  tid   = omp_get_thread_num()           // my thread ID
  lsize = int((kend-kst+1)/nthrds)+1     // junk size

  kf = tid*lsize + kst                   // index range for this thread
  kl = min(((tid+1)*lsize + kst - 1),kend)
  kp = 1                                 // first forward direction
  do nswz = 1,2
    do k = kf, kl, kp                    //  plain k
       .....
       app(i,j,k)  = ....                //  cube data
    end do

    kp = -kp                             // reverse direction
  end do
```



shm: system solve - speedup

#threads	PROGRAM	SOLVE	MECFLU	SIMPLE	CALPH
1	298	85	186	30	51
2	188	54	116	20	32
4	101	28	63	12	17
6	73	18	45	9.2	10
8	61	15	37	8.6	66
12	47	10	27	8.6	7.5
speedup	**6.3**	**8.4**	6.8	**3.6**	6.7

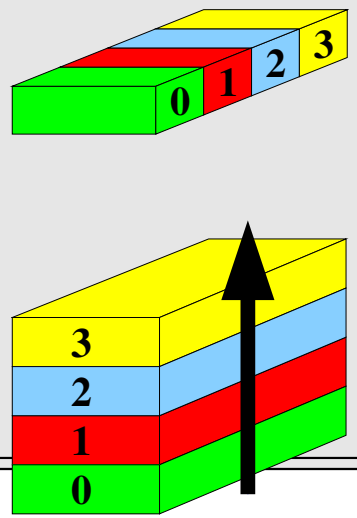
Speedup on dualhex, time in min.

- good speedup of 8.4 in SOLVE
- poor speedup of 3.6 in SIMPLE
  - unnecessary reduce directive for an array (OpenMP 3.0)
  - extra parallel–loop for boundary data $\Longrightarrow$ data shuffling
- speedup of 6.7 in update (vectors and material coeff.) can be further improved by avoiding above data shuffling

Listing 9: Handling of boundary data (shuffling)

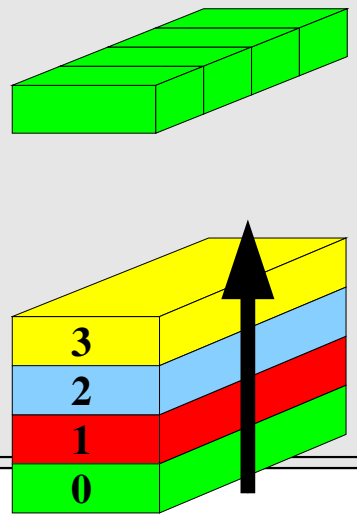
```
...
 !$omp parallel do shared(app) schedule(static)
    do j=1,N                          // lines in plane
       ....
       app(i,j,1) += ....             // boundary data in plain 1
    end do


                                      // data shuffling !!!!!!!
 !$omp parallel do shared(app) schedule(static)
    do k=1,N                          // plain k
       .....
       app(i,j,k) += ....             // cube data
    end do
...
```



Listing 10: Handling of boundary data (no shuffling)

```
...
!$omp parallel shared(app) schedule(static)
tid = omp_get_thread_num()
if (tid .EQ. 0)              // app(*,*,1)  stored on thread 0
   do j=1,N
      ....
      app(i,j,1) += ....     // boundary data
   end do
end if
                             //  no data shuffling
!$omp do
   do k=1,N                  //  plain k
      .....
      app(i,j,k) += ....     //  cube data
   end do
...
```



shm: system solve - Aug. 2011

#threads	PROGRAM	SOLVE	MECFLU	SIMPLE	CALPH
speedup July'11	**6.3**	**8.4**	6.8	**3.6**	6.7
speedup Aug'11	**11.7**	**11.4**	11.8	**11.3**	11.1

dualhex: Speedup with 12 threads

- no reduce arrays (SIMPLE)
- sequential handling of boundary data (no data shuffling)
- **temp. data** are always **private** (MECFLU)!
- no dynamic memory allocation in threads
- larger scope for #pragma omp parallel (PRAGMA)
- beware of **data race** in **loop dependencies** ($\downarrow$) for pre-computed data

Nov. 2013: 4-year project in Chile for D. Vasco

shm: pitfall for polynom: $p = \sum_{k=0}^{N} a_k \cdot x^k$

Listing 11: Polynom sequentially

```
  p  = 0.0
  xk = 1.0
  do k = 1, N+1
     p  = p + a(k)*xk      ! add   a_k * x^k
     xk = xk*x
  end do
```

Listing 12: Polynom shm (wrong result)

```
  p  = 0.0
  xk = 1.0
!$omp parallel do private(k) shared(xk,a) reduction(+:p)
  do k = 1, N+1
     p  = p + a(k)*xk
     xk = xk*x             ! dependency between loops
  end do
```

shm: correct for polynom

$$p = \sum_{k=0}^{N} a_k \cdot x^k = \sum_{\text{tid}=0}^{\text{nthrds-1}} \sum_{k=kf_{\text{tid}}}^{kl_{\text{tid}}} a_k \cdot x^k$$

Calculate for thread `tid` its index range `[kf,kl]` explicitely.

Listing 13: Polynom shm

```
  p  = 0.0
!$omp parallel private(k,xk) shared(a) reduction(+:p)
  nthrd = omp_get_num_threads() ! number of threads
  tid   = omp_get_thread_num()  ! my thread number
  lsize = int((N+1)/nthrds)+1   ! my max. portion of data
  kf    = tid*lsize+1           ! interval
  kl    = min(kf+lsize, N+1)
  xk = x**(kf-1)                ! correct x^k for this thread
  do k = kf, kl
     p  = p + a(k)*xk
     xk = xk*x
  end do
!$omp parallel                  ! correct result
```

Examples: programming environment

Getting the code

- Download code (link)
- unzip: `> tar xzf Chile.tgz`
- change into an environment *shm*: `> cd shm`
- change into a subdirectory: `> cd skalar`
- compile, link and run: `> make run`

Each directory contains at least *skalar* and jacobi, partially also with its MPI paralleliazion therein.

- `> cd shm; ls *default.mk` lists all supported compilers (here: GCC_ , ICC_ , PGI_)
- `> cd skalar; make COMPILER=ICC_ run` uses the Intel-compiler.

Supported parallel environments

- Sequential in directory *seq*.
- OpenMP 3.0 in directory *shm*.
- MPI in directory *par*.
- CUDA in directory *CUDA*.
- OpenACC in directory *OpenACC*.
- MIC (MIC-pragmas / OpenMP 4.0) in directory *MIC*.
- MPI+OpenMP in directory *OpenACC/par**.
- MPI+CUDA in *CUDA/par**.
- MPI+OpenACC in *OpenACC/par**: