



# Numerical Simulation of Elastic Waves in 3D using FFT algorithm and MPI protocol

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# Outline

Introduction

**Case study: simulation of earthquake motion in 3D**

Numerical solution of the wave equation

**Fourier method**

**FFT algorithm**

Parallel implementation with MPI

**Domain decomposition I**

**Domain decomposition II**

Introduction to the Lab Session (this afternoon)

**Elastic waves propagation in 2D (with dom. dec. I)**



# Simulation of earthquake ground motion

## Purpose:

Improve seismic hazard assessment in sites with

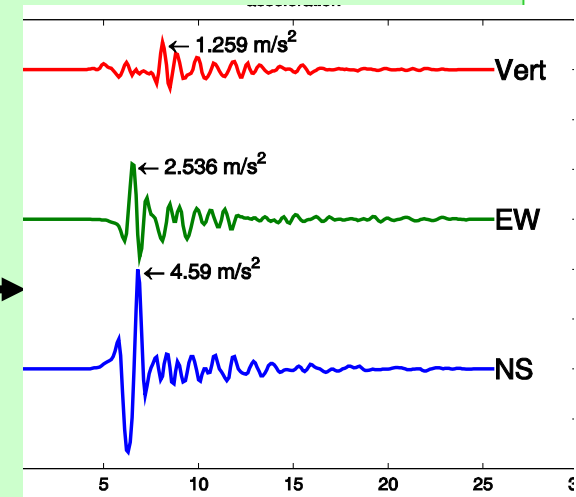
- lacking empirical ground motion data (past earthquakes)
- complex geology

# Simulation of earthquake ground motion

## Method:

Numerical simulation based on:

- seismic source model (wave generation)
- geological structure model (wave propagation)



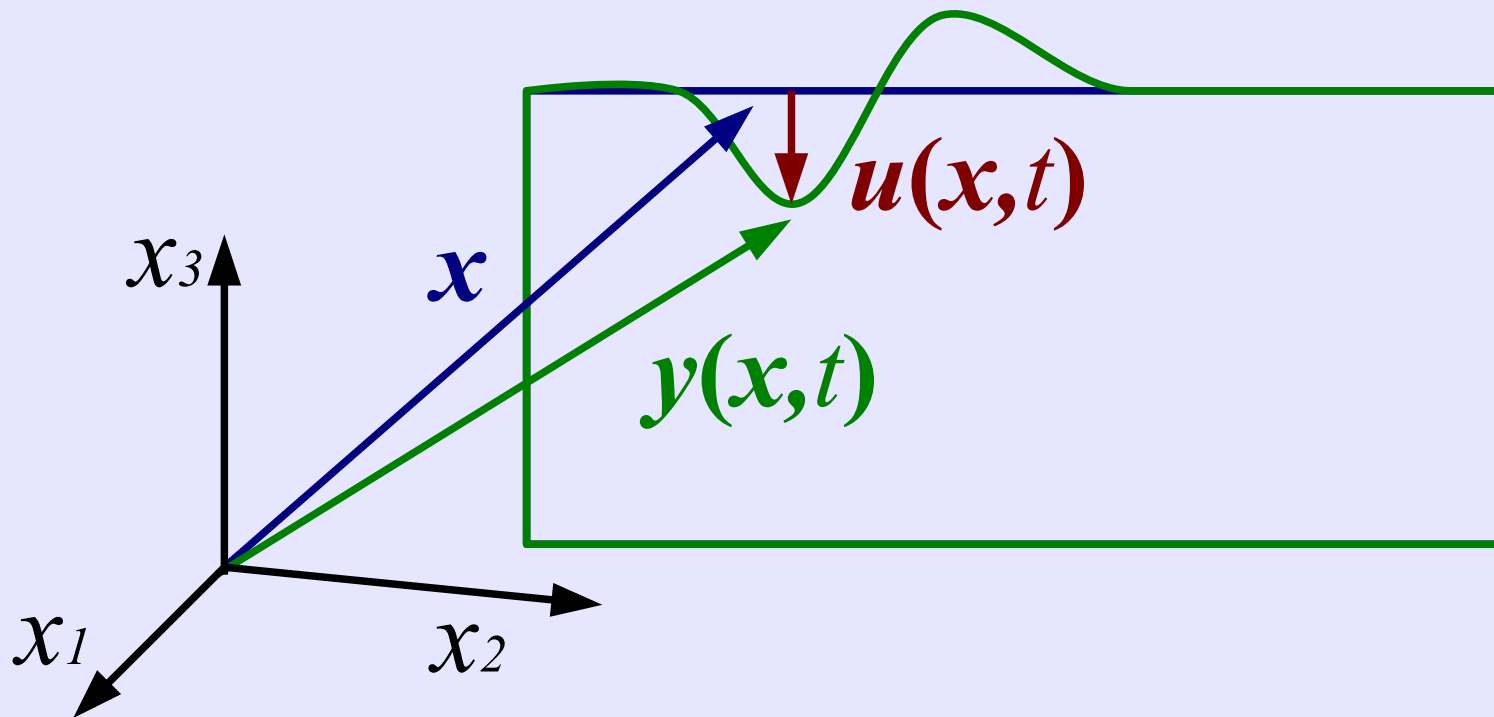
$$u(x, t) = s(t) * G(x, t)$$

Green's function

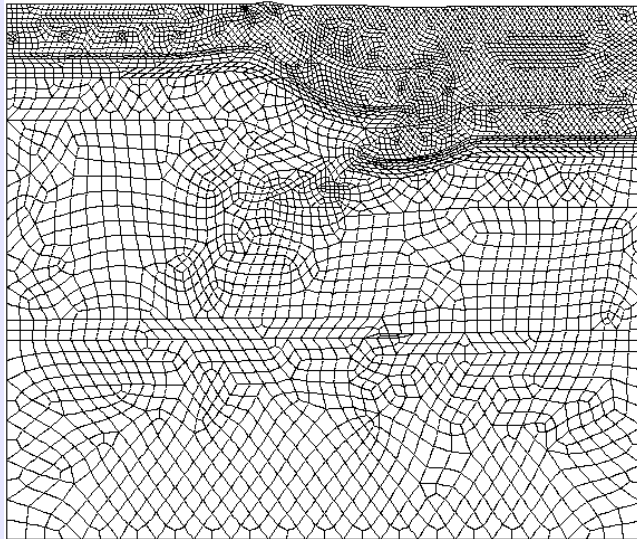
# Simulation of earthquake ground motion

Physical quantity:

**Displacement:**  $u(\mathbf{x}, t) = \mathbf{y}(\mathbf{x}, t) - \mathbf{x}$  continuous and differentiable!

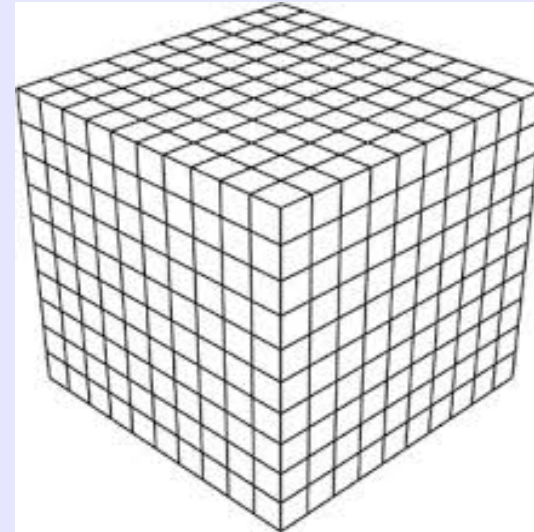


# Spatial discretization



## Unstructured grid

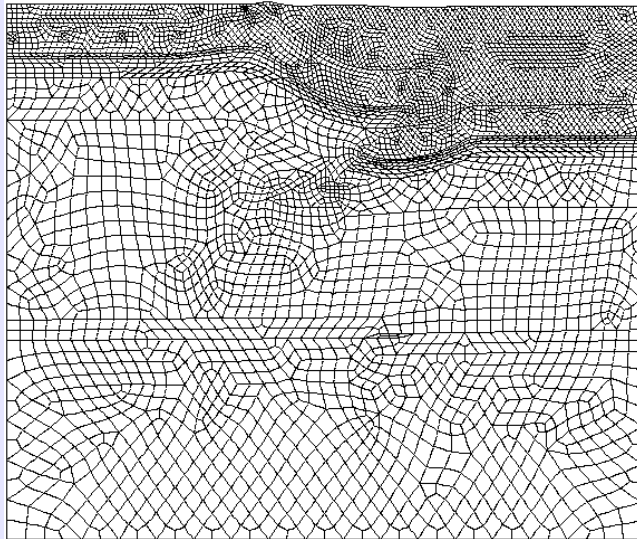
variational formulation  
(spatial integrals)



## Structured grid

variational formulation  
&  
differential formulation  
(spatial derivatives)

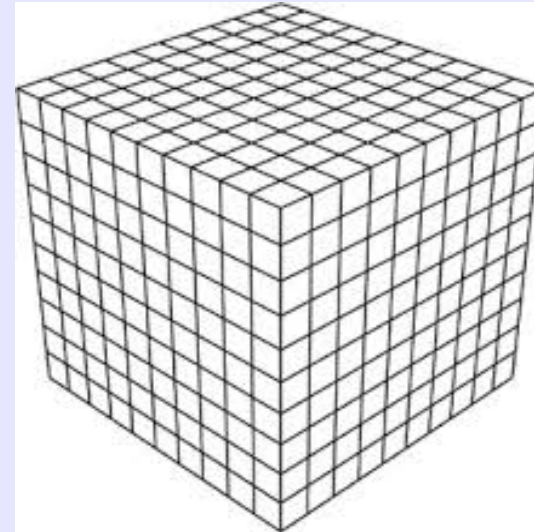
# Spatial discretization



Unstructured grid

**very flexible**

**sophisticated for 3D**



Structured grid

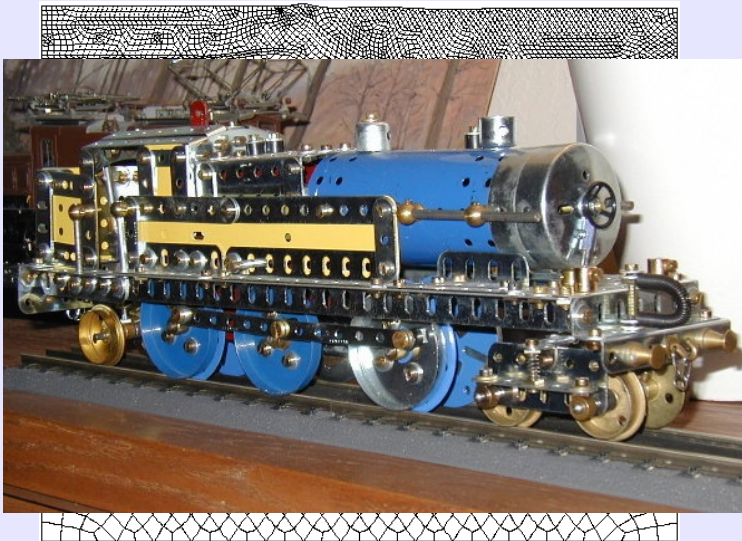
**less flexible**

**simple**



# Spatial discretization

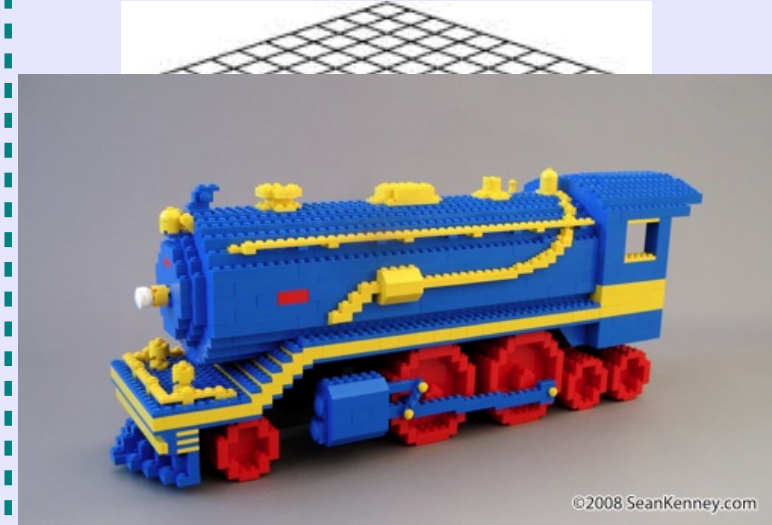
Our choice



Unstructured grid

very flexible

sophisticated for 3D



Structured grid

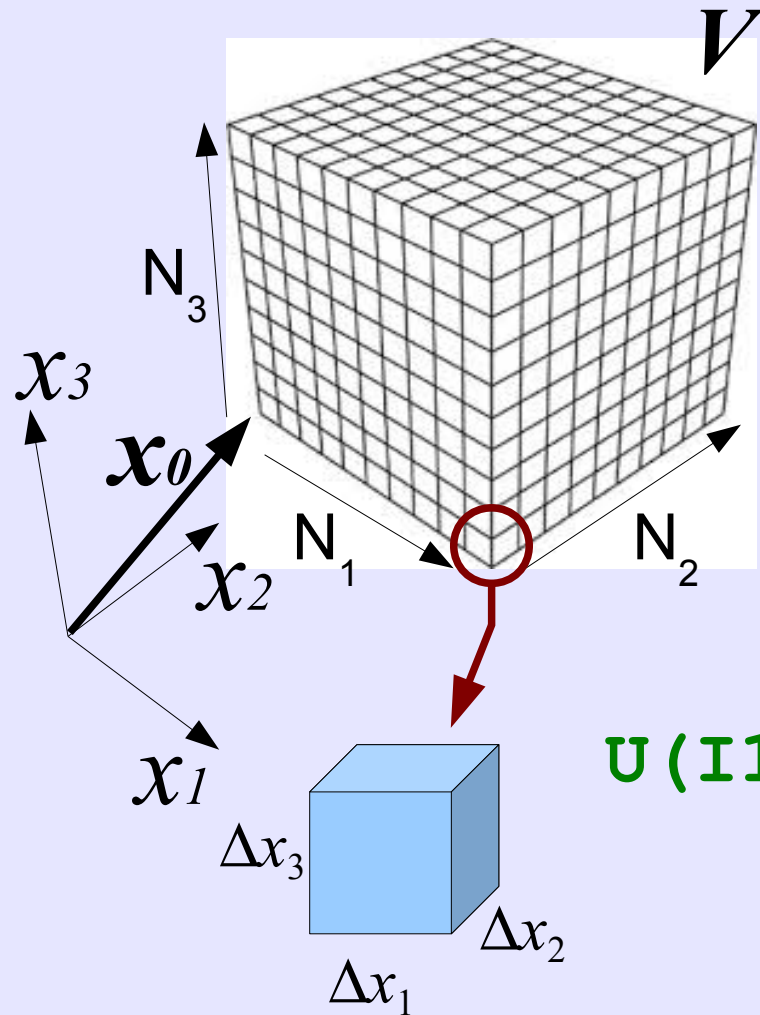
less flexible

simple





# Spatial discretization



Physical variable:

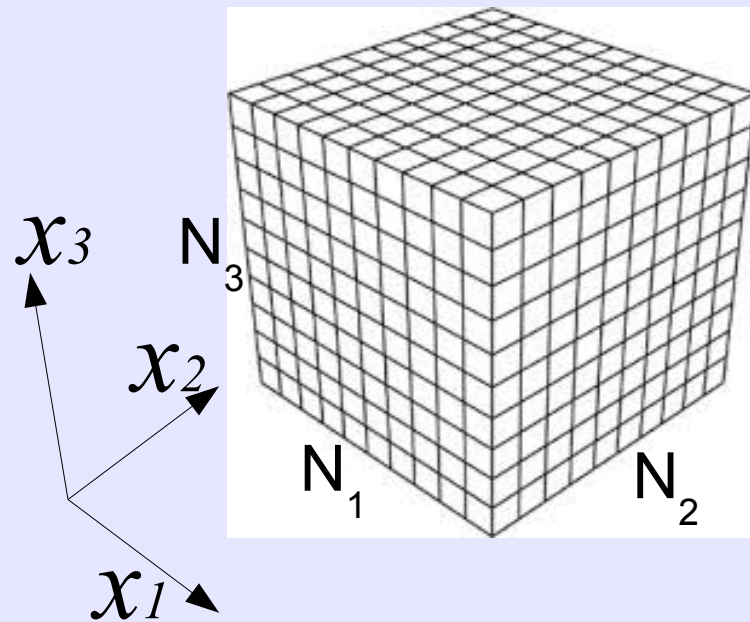
$$u(\mathbf{x}) : V \subset \mathbb{R}^3 \rightarrow \mathbb{R}^3$$

Numerical variable (FORTRAN):

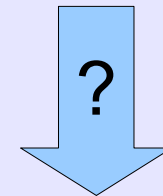
`REAL, DIMENSION (N1, N2, N3, 3) :: U`

$$U(I1, I2, I3, IC) = u_{ic}(\mathbf{x}_0 + (i_1 \Delta x_1, i_2 \Delta x_2, i_3 \Delta x_3))$$

# Spatial derivatives in structured grid



$$U(N_1, N_2, N_3) \longrightarrow u(x_1, x_2, x_3)$$

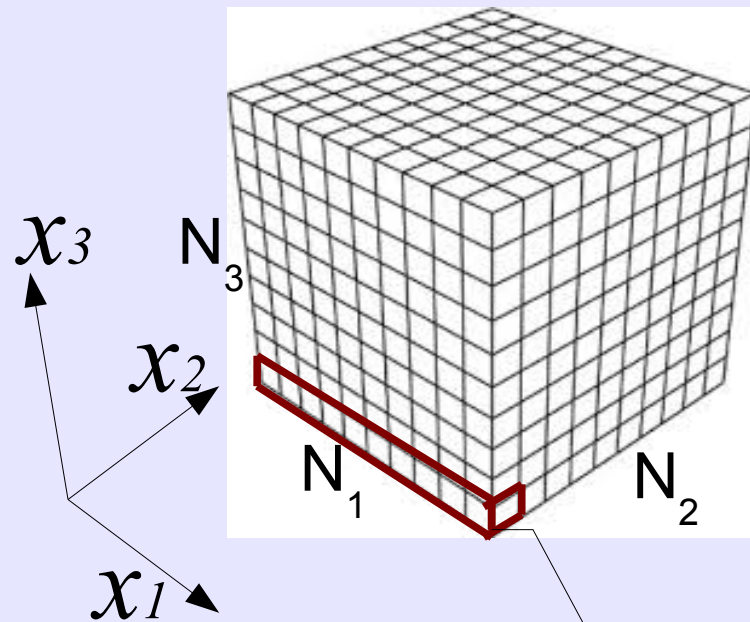


$$D1U(N_1, N_2, N_3) \longrightarrow \partial_1 u(x_1, x_2, x_3)$$

$$D2U(N_1, N_2, N_3) \longrightarrow \partial_2 u(x_1, x_2, x_3)$$

$$D3U(N_1, N_2, N_3) \longrightarrow \partial_3 u(x_1, x_2, x_3)$$

# Spatial derivatives in structured grid



$$U(N_1, N_2, N_3) \longrightarrow u(x_1, x_2, x_3)$$

?

$$D1U(N_1, N_2, N_3) \longrightarrow \partial_1 u(x_1, x_2, x_3)$$

$$D2U(N_1, N_2, N_3) \longrightarrow \partial_2 u(x_1, x_2, x_3)$$

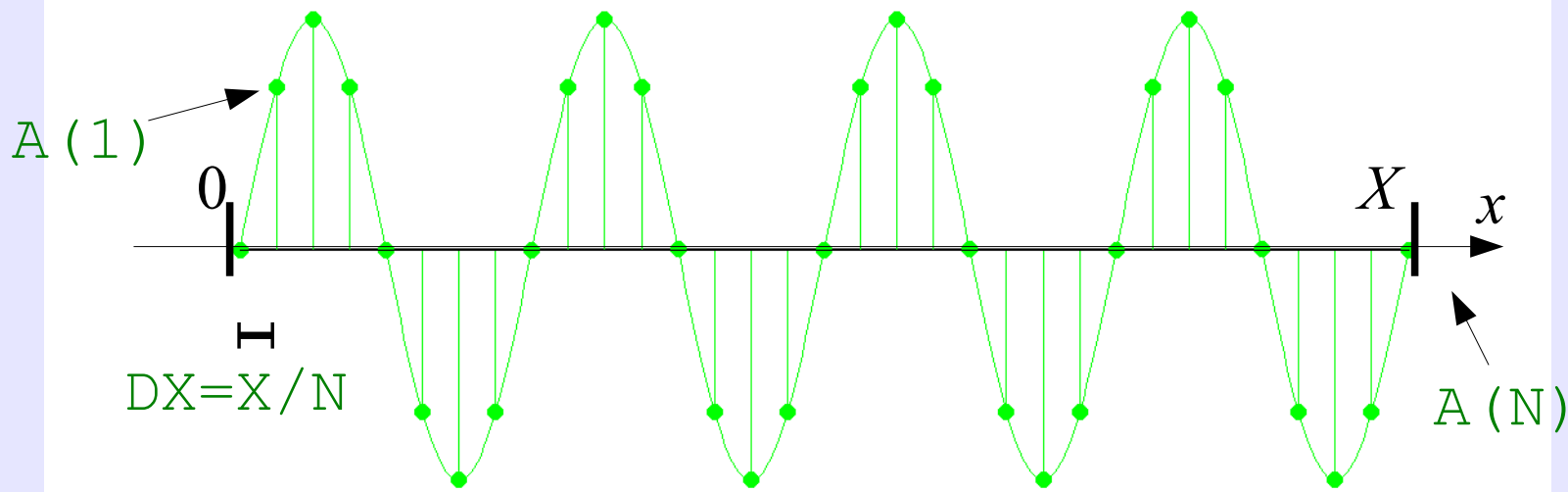
$$D3U(N_1, N_2, N_3) \longrightarrow \partial_3 u(x_1, x_2, x_3)$$

$$A = U(1:N_1, 1, 1)$$

?

$$DA(1:N_1)$$

# Spatial derivatives with the Fourier method



$$A(I) = C * \text{SIN}(W * I); \quad I=1, 2, \dots, N$$

REAL :: C

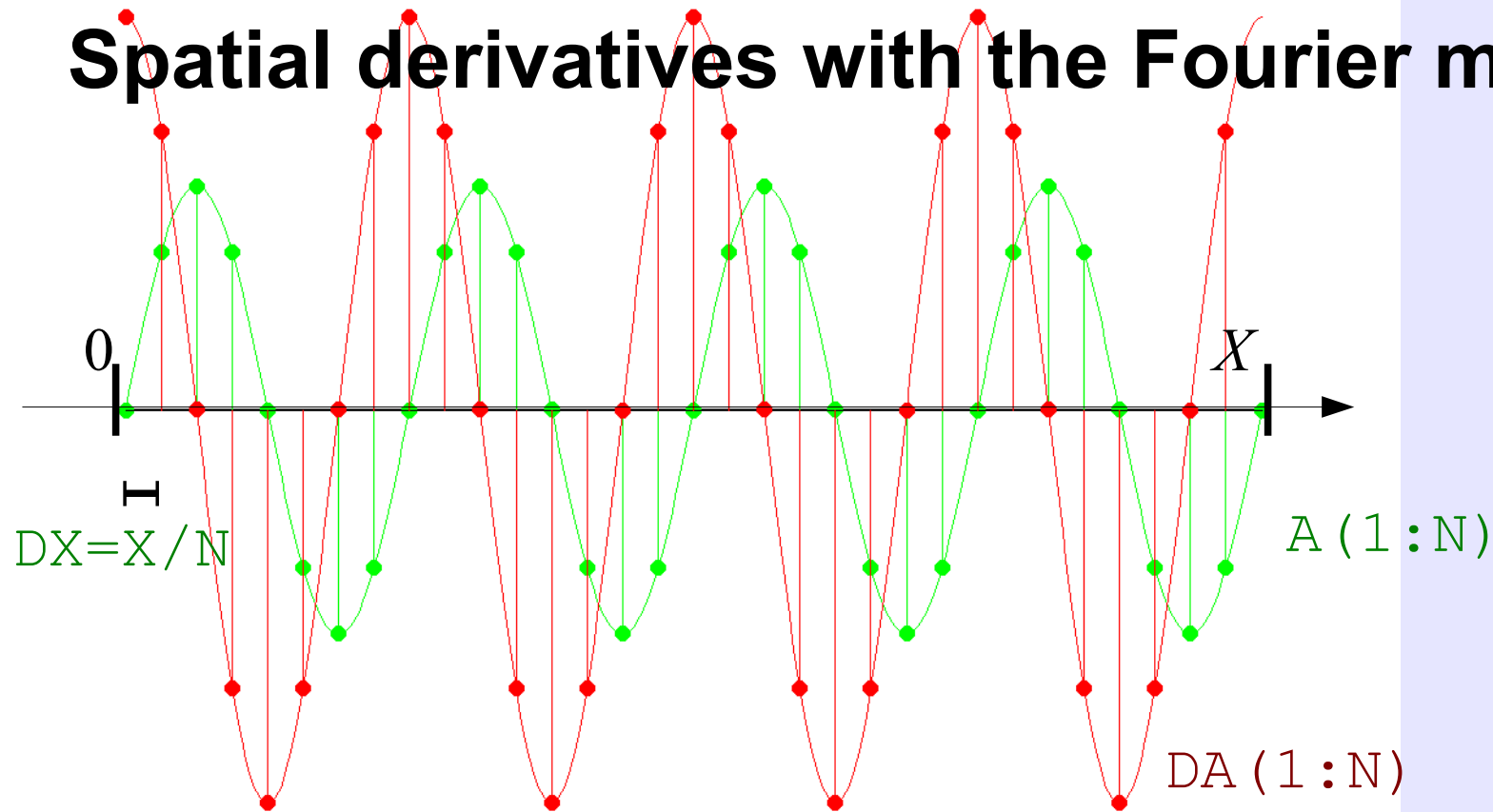
REAL :: W = J \* 2 \* PI / N !

J.GE.0 & J.LT.N

Nyquist  
criterion



# Spatial derivatives with the Fourier method



$$A(I) = C * \text{SIN}(W * I); \quad I=1, 2, \dots, N$$

$$DA(I) = W * C * \text{COS}(W * I) / DX; \quad I=1, 2, \dots, N$$

**EXACT!**

# Spatial derivatives with the Fourier method

...

```
REAL, DIMENSION(N) :: A, DA
```

```
REAL, PARAMETER :: DX=X/REAL(N)
```

```
REAL, PARAMETER :: W= J*2*PI/N !J.GE.0 & J.LT.N
```

```
REAL :: C
```

$$A(I) = C * \sin(W * I) \quad \longrightarrow \quad DA(I) = W * C * \cos(W * I) / DX$$

$$A(I) = C * \cos(W * I) \quad \longrightarrow \quad DA(I) = -W * C * \sin(W * I) / DX$$

$$I=1, 2, \dots, N$$

# Spatial derivatives with the Fourier method

...

**COMPLEX, DIMENSION (N) :: A, DA**

**COMPLEX, PARAMETER :: AI = CMPLX(0.0, 1.0)**

**REAL, PARAMETER :: DX=X/REAL(N)**

**REAL, PARAMETER :: W= J\*2\*PI/N**

**COMPLEX :: C**

$$A(I) = C * \text{EXP}(AI * W * I) \longrightarrow DA(I) = C * AI * W * \text{EXP}(AI * W * I) / DX$$

$$I = 1, 2, \dots, N$$

$$\exp(i\phi) = \sin(\phi) + i \cos(\phi)$$

# Spatial derivatives with the Fourier method

```

COMPLEX, DIMENSION (N) :: A, DA
COMPLEX :: AI = CMPLX(0.0, 1.0)
REAL, PARAMETER :: DX=X/REAL(N)
REAL, DIMENSION (N), PARAMETER :: W=(J*2*PI/N, J=0, N-1)
COMPLEX, DIMENSION (N) :: C !DEFINED SOMEHOW
  
```

$$A(I) = \text{SUM}(C(:) * \text{EXP}(AI * W(:) * I))$$



$$DA(I) = \text{SUM}(AI * W(:) * C(:) * \text{EXP}(AI * W(:) * I)) / DX$$

$$I=1, 2, \dots, N$$

$$\partial_x \left[ \sum_n c_n \exp(i k_n x) \right] = \sum_n i k_n c_n \exp(i k_n x)$$



# Spatial derivatives with the Fourier method

```

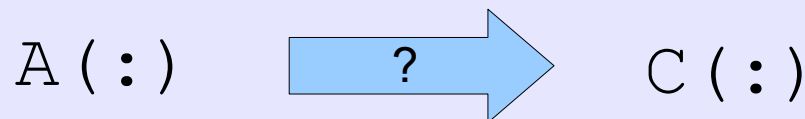
COMPLEX, DIMENSION (N) :: A, DA
COMPLEX :: AI = CMPLX(0.0, 1.0)
REAL, PARAMETER :: DX=X/REAL(N)
REAL, DIMENSION(N), PARAMETER:: W=(J*2*PI/N, J=0, N-1)
COMPLEX, DIMENSION(N) :: C
  
```

$$A(I) = \text{SUM}(C(:) * \text{EXP}(AI * W(:) * I))$$



$$DA(I) = \text{SUM}(AI * W(:) * C(:) * \text{EXP}(AI * W(:) * I)) / DX$$

$I=1, 2, \dots, N$



# Spatial derivatives with the Fourier method

COMPLEX, DIMENSION (N) :: A, DA

COMPLEX :: AI = CMPLX(0.0, 1.0)

REAL, PARAMETER :: DX=X/REAL(N)

REAL, DIMENSION(N), PARAMETER :: W=(J\*2\*PI/N, J=0, N-1)

COMPLEX, DIMENSION(N) :: C

**Discrete  
Fourier  
Transform**

$$C(I) = \text{SUM}(A(:) * \text{EXP}(-AI * W(:) * I))$$

$I=1, 2, \dots, N$

$$A(I) = \text{SUM}(C(:) * \text{EXP}(AI * W(:) * I)) / N$$

$I=1, 2, \dots, N$

**Inverse  
Discrete  
Fourier  
Transform**

# Spatial derivatives with the Fourier method

COMPLEX, DIMENSION (N) :: **A**, **DA**

COMPLEX, DIMENSION (N) :: **AIW**

**AIW**=CMPLX ( 0 . 0 , ( J\*2\*PI/N, J=0, N-1 ) )

**DA**=**IDFT** ( **AIW**\***DFT** ( **A** ) ) / ( N\*DX )

Dynamic meteorology and oceanography (Kreiss & Oliger, 1973)

2D acoustic waves (Gazdag 1981)

2D elastic waves (Kosloff et al. 1984)

# Spatial derivatives with the Fourier method

COMPLEX, DIMENSION (N) :: **A**, **DA**

COMPLEX, DIMENSION (N) :: **AIW**

**AIW**=CMPLX ( 0.0, ( J\*2\*PI/N, J=0, N-1) )

**DA**=**IDFT** ( **AIW**\***DFT** ( **A** ) ) / ( N\*DX )

```
FUNCTION IDFT (C)
DO I=1,N
  IDFT(I)=SUM( C(:) * EXP(AIW(:)*I) )
ENDDO
```

```
FUNCTION DFT (A)
DO I=1,N
  DFT(I)=SUM( A(:) * EXP(-AIW(:)*I) )
ENDDO
```

# Spatial derivatives with the Fourier method

```
COMPLEX, DIMENSION (N) :: A, DA
```

```
COMPLEX, DIMENSION (N) :: AIW
```

```
AIW=CMPLX (0.0, (J*2*PI/N, J=0, N-1))
```

```
DA=IDFT (AIW*DFT (A) ) / (N*DX)
```

```
FUNCTION IDFT (C)  
DO I=1,N  
  IDFT(I)=SUM( C(:) * EXP(AIW(:)*I)  
ENDDO
```

```
FUNCTION DFT (A)  
DO I=1,N  
  DFT(I)=SUM( A(:) * EXP(-AIW(:)*I)  
ENDDO
```

runtime =  $O(N^2)$

NOT for HPC !

# Fast Fourier Transform (FFT)

- many different algorithms for evaluating DFT
- runtime improvement from  $O(N^2)$  to  $O(N \log_2 N)$
- complex & real data
- several libraries and packages (FFTPACK, FFTW... )



OK for  
HPC!

**Use always FFT, never implement DFT**

For more details see last week Gavin Pringle presentation:

<http://indico.ictp.it/event/a13229/session/8/contribution/35/material/0/1.pdf>

## Spatial derivatives using FFTW3

```
INCLUDE 'fftw3.f'  
COMPLEX, DIMENSION (N) :: A, DA  
COMPLEX, DIMENSION (N) :: AIW=&  
                                CMPLX (0.0, (J*2*PI/N, J=0, N-1)) / (N*DX)  
COMPLEX, DIMENSION (N) :: C  
INTEGER*8, DIMENSION (2) :: I8PLAN
```

```
CALL SFFTW_PLAN_DFT_1D (I8PLAN (1), &  
                        N, A, C, FFTW_FORWARD, FFTW_ESTIMATE)
```

*Setup FFT*

```
CALL SFFTW_PLAN_DFT_1D (I8PLAN (2), &  
                        N, C, DA, FFTW_BACKWARD, FFTW_ESTIMATE)
```

```
CALL SFFTW_EXECUTE_DFT (I8PLAN (1), A, C)  
C=C*AIW  
CALL SFFTW_EXECUTE_DFT (I8PLAN (2), C, DA)
```

*Apply FFT*

# Additional speed up with FFT

## 1) Buy one & get one free



```
REAL, DIMENSION (N, 2) :: U  
COMPLEX, DIMENSION (N) :: A, DA
```

```
A = CMPLX (U (1:N, 1), U (1:N, 2))
```

```
DA=IFFT (AIW*FFT (A))
```

```
D1U (1:N, 1) =REAL (DA)  
D1U (1:N, 2) =AIMAG (DA)
```



## Additional speed up with FFT

### 2) From real to complex and back ( $N$ even )

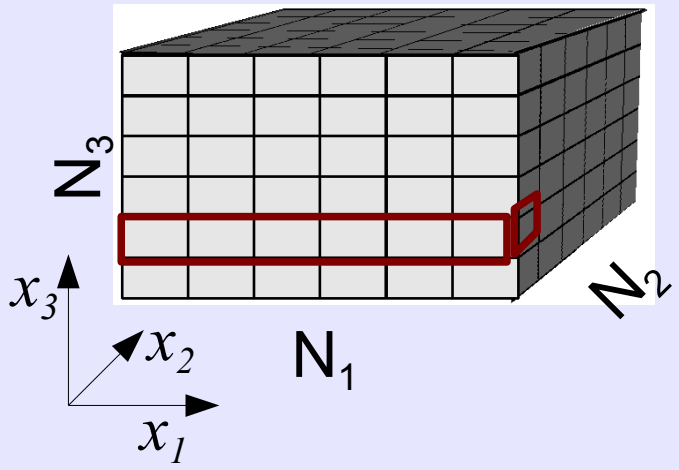


```
REAL, DIMENSION(N) :: U, DU  
COMPLEX, DIMENSION(N/2+1) :: C, AIW
```

```
C=FFT_R2C(U)  
DU=FFT_C2R(AIW*C)
```

**FFT\_R2C & FFT\_C2R**  
(almost) half less expensive  
than FFT

# Spatial derivatives with FFT in a volume



$U(1:N1, 1:N2, 1:N3)$

$\rightarrow D1U(1:N1, 1:N2, 1:N3)$

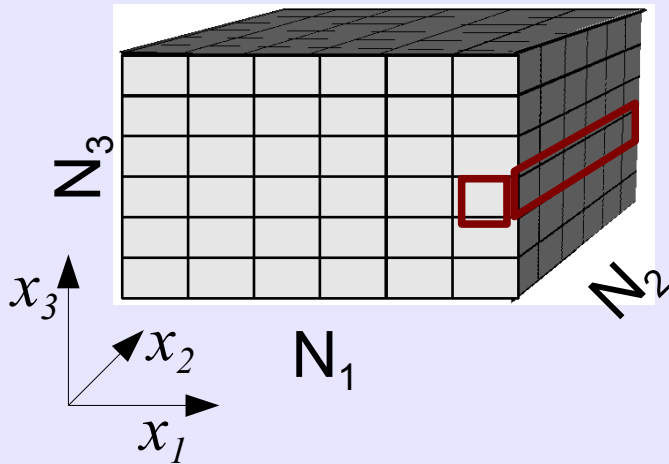
```

    graph TD
      A[Loop I3 from 1 to N3] --> B[Loop I2 from 1 to N2]
      B --> C["C=FFT_R2C(U(:, I2, I3))"]
      C --> D["D1U(:, I2, I3)=FFT_C2R(AIW1*C)"]
      D --> E(( ))
      E --> B
      E --> A
  
```

Runtime

$N3 * N2 * N1 * (1 + 2 * \log_2(N1))$

# Spatial derivatives with FFT in a volume



$U(1:N1, 1:1:N2, 1:N3)$

$\rightarrow D2U(1:N1, 1:N2, 1:N3)$

Loop I3 from 1 to N3

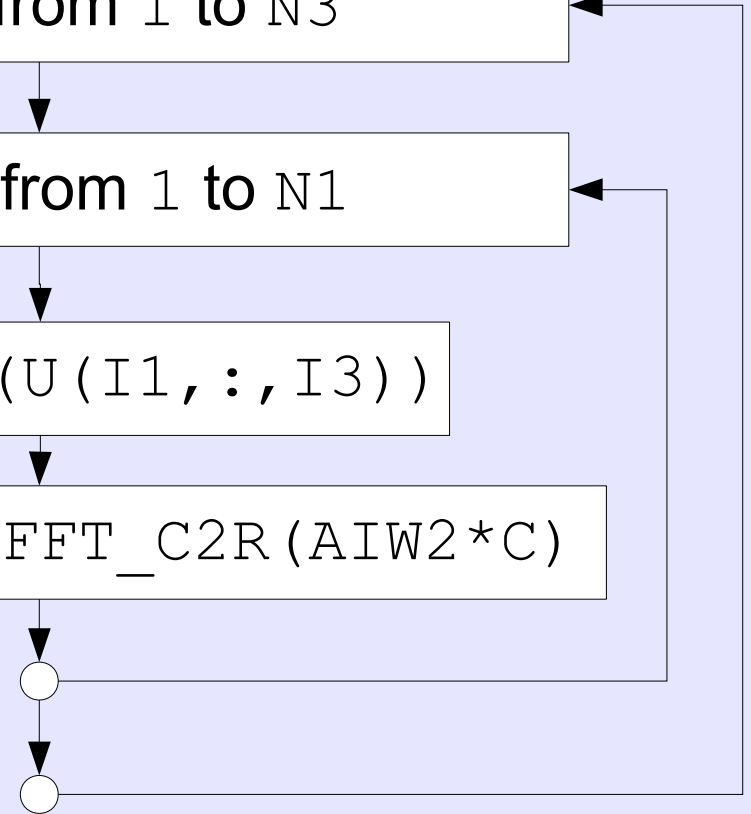
Loop I1 from 1 to N1

$C = \text{FFT\_R2C}(U(I1, :, I3))$

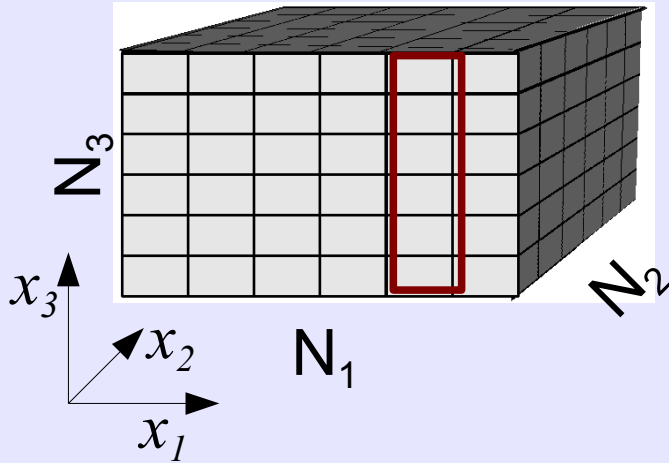
$D2U(I1, :, I3) = \text{FFT\_C2R}(AIW2 * C)$

Runtime

$N3 * N2 * N1 * (1 + 2 * \log_2(N2))$

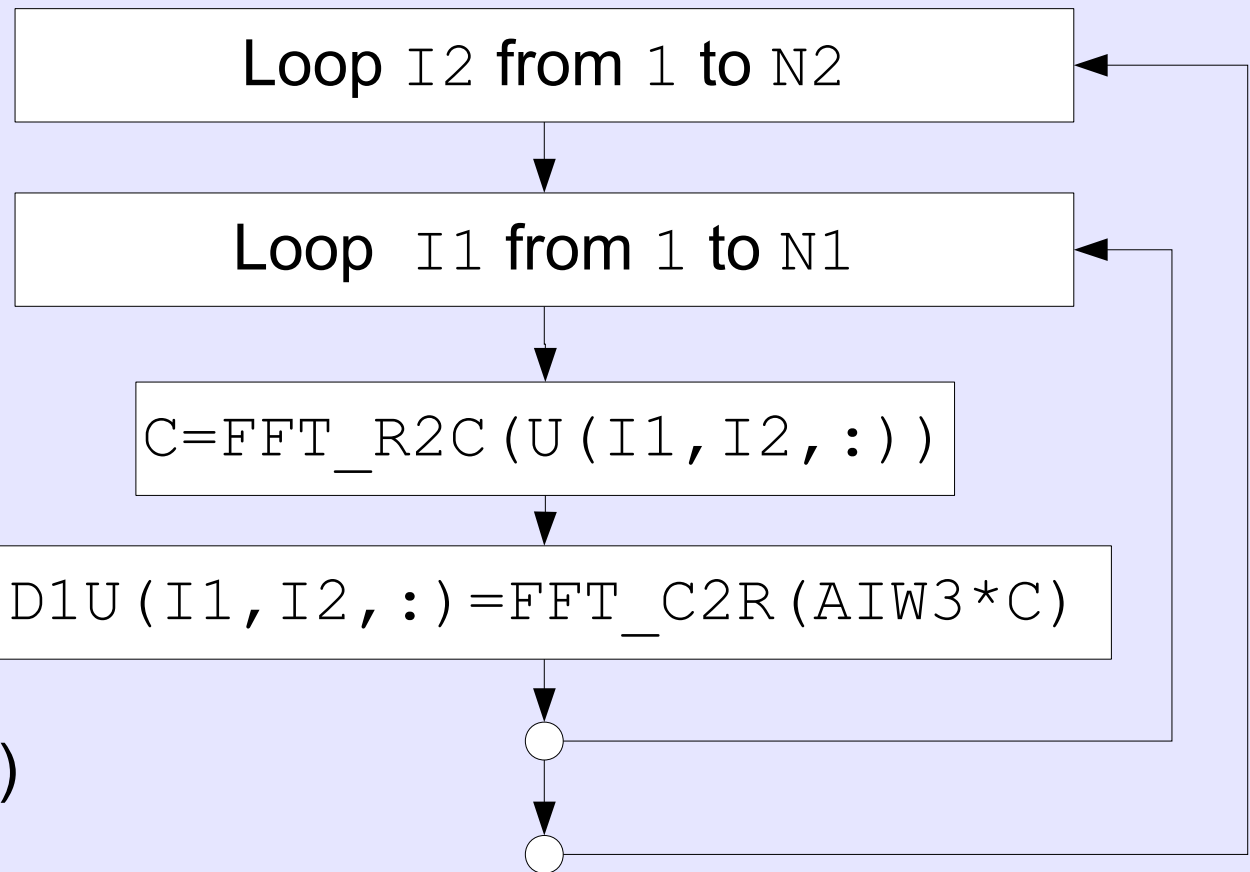


# Spatial derivatives with FFT in a volume



$U(1:N1, 1:1:N2, 1:N3)$

$\rightarrow D3U(1:N1, 1:N2, 1:N3)$



Runtime

$N_3 * N_2 * N_1 * (1 + 2 * \log_2(N_3))$

# Elastic waves

$$\partial_{tt} \mathbf{u} = \rho^{-1} \left( \nabla \left[ \mathbf{C} \nabla^T \mathbf{u} \right] + \mathbf{f} \right) \quad \text{Equation of motion}$$

Displacement vector

$$\mathbf{u} = \left( u_1, u_2, u_3 \right)^T$$

Auld's differential operator

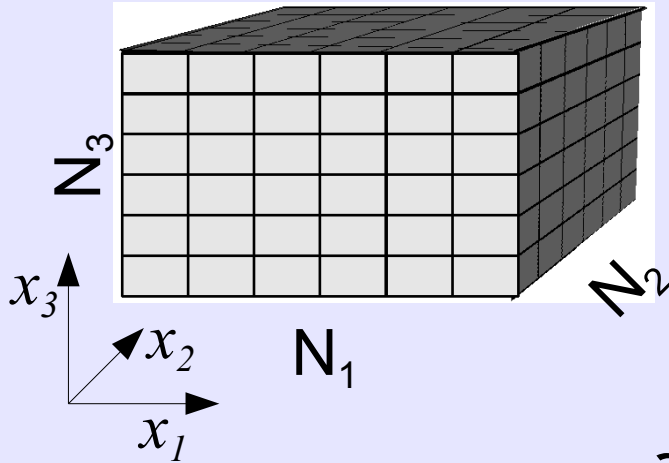
$$\nabla = \begin{pmatrix} \partial_1 & 0 & 0 & 0 & \partial_3 & \partial_2 \\ 0 & \partial_2 & 0 & \partial_3 & 0 & \partial_1 \\ 0 & 0 & \partial_3 & \partial_2 & \partial_1 & 0 \end{pmatrix}$$

Elasticity matrix:

$$\mathbf{C} = \begin{pmatrix} c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} \\ c_{12} & c_{22} & c_{23} & c_{24} & c_{25} & c_{26} \\ c_{13} & c_{23} & c_{33} & c_{34} & c_{35} & c_{36} \\ c_{14} & c_{24} & c_{34} & c_{44} & c_{45} & c_{46} \\ c_{15} & c_{25} & c_{35} & c_{45} & c_{55} & c_{56} \\ c_{16} & c_{26} & c_{36} & c_{46} & c_{56} & c_{66} \end{pmatrix}$$

$\partial_1, \partial_2, \partial_3$  :  
partial derivatives  
in the 3 spatial directions

# Computational cost



$$\partial_{tt} \mathbf{u} = \rho^{-1} \left( \nabla \left[ \mathbf{C} \nabla^T \mathbf{u} \right] + \mathbf{f} \right)$$

$\partial_1$	6 * N3*N2*N1*(1+2*log2(N1)) +
$\partial_2$	6 * N3*N2*N1*(1+2*log2(N2)) +
$\partial_3$	6 * N3*N2*N1*(1+2*log2(N3)) +
Constants multiplication	6 * N3*N2*N1*12
	=

$$\text{Runtime: } 6*N*(15+2*\log_2(N))$$

$$N=N3*N2*N1$$

## Recasting 2nd order as 1st order

$$\begin{cases} \partial_{tt} \mathbf{u}(\mathbf{x}, t) = \mathbf{F}(t, \mathbf{u}(\mathbf{x}, t)) \\ \partial_t \mathbf{u}(\mathbf{x}, 0) = \dot{\mathbf{u}}_0 \\ \mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0 \end{cases}$$

## Recasting 2nd order as 1st order

$$\begin{cases} \partial_{tt} \mathbf{u}(\mathbf{x}, t) = \mathbf{F}(t, \mathbf{u}(\mathbf{x}, t)) \\ \partial_t \mathbf{u}(\mathbf{x}, 0) = \dot{\mathbf{u}}_0 \\ \mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0 \end{cases}$$

$$\begin{cases} \partial_t \mathbf{u}(\mathbf{x}, t) = \mathbf{v}(\mathbf{x}, t) \\ \partial_t \mathbf{v}(\mathbf{x}, t) = \mathbf{F}(t, \mathbf{u}(\mathbf{x}, t)) \\ \mathbf{v}(\mathbf{x}, 0) = \dot{\mathbf{u}}_0 \\ \mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0 \end{cases}$$



## Recasting 2nd order as 1st order

$$\begin{cases} \partial_{tt} \mathbf{u}(\mathbf{x}, t) = \mathbf{F}(t, \mathbf{u}(\mathbf{x}, t)) \\ \partial_t \mathbf{u}(\mathbf{x}, 0) = \dot{\mathbf{u}}_0 \\ \mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0 \end{cases}$$

$$\begin{cases} \partial_t \mathbf{u}(\mathbf{x}, t) = \mathbf{v}(\mathbf{x}, t) \\ \partial_t \mathbf{v}(\mathbf{x}, t) = \mathbf{F}(t, \mathbf{u}(\mathbf{x}, t)) \\ \mathbf{v}(\mathbf{x}, 0) = \dot{\mathbf{u}}_0 \\ \mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0 \end{cases}$$

$$\mathbf{Y} = \begin{bmatrix} \mathbf{u} \\ \mathbf{v} \end{bmatrix} ; \quad \tilde{\mathbf{F}} = \begin{bmatrix} 1 \\ \mathbf{F} \end{bmatrix} \quad \longrightarrow$$

$$\begin{cases} \partial_t \mathbf{Y}(\mathbf{x}, t) = \tilde{\mathbf{F}}(\mathbf{x}, t) \\ \mathbf{Y}(\mathbf{x}, 0) = \mathbf{Y}_0 \end{cases}$$

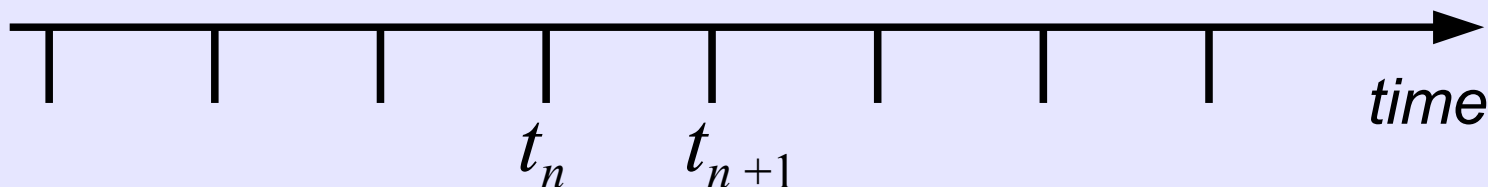
## Explicit one step time integration

$$\begin{cases} \partial_t Y(\mathbf{x}, t) = F(\mathbf{x}, t) \\ Y(\mathbf{x}, 0) = Y_0 \end{cases}$$

Discretization of the time axis

$$t_{n+1} = t_n + \Delta t \quad \forall n \in \{0, 1, \dots, N\}$$

$\Delta t$  respects some criteria  
(not discussed here)

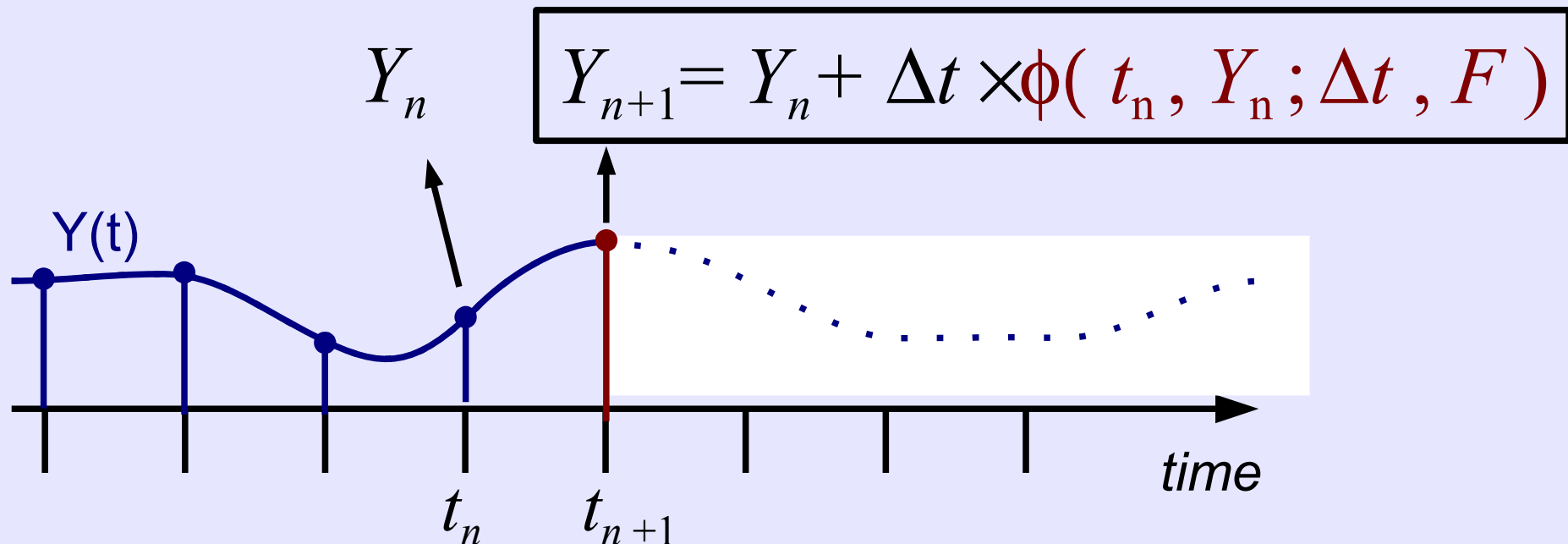


## Explicit one step time integration

$$\begin{cases} \partial_t Y(\mathbf{x}, t) = F(\mathbf{x}, t) \\ Y(\mathbf{x}, 0) = Y_0 \end{cases}$$

Discretization of the time axis

$$t_{n+1} = t_n + \Delta t \quad \forall n \in \{0, 1, \dots, N\}$$

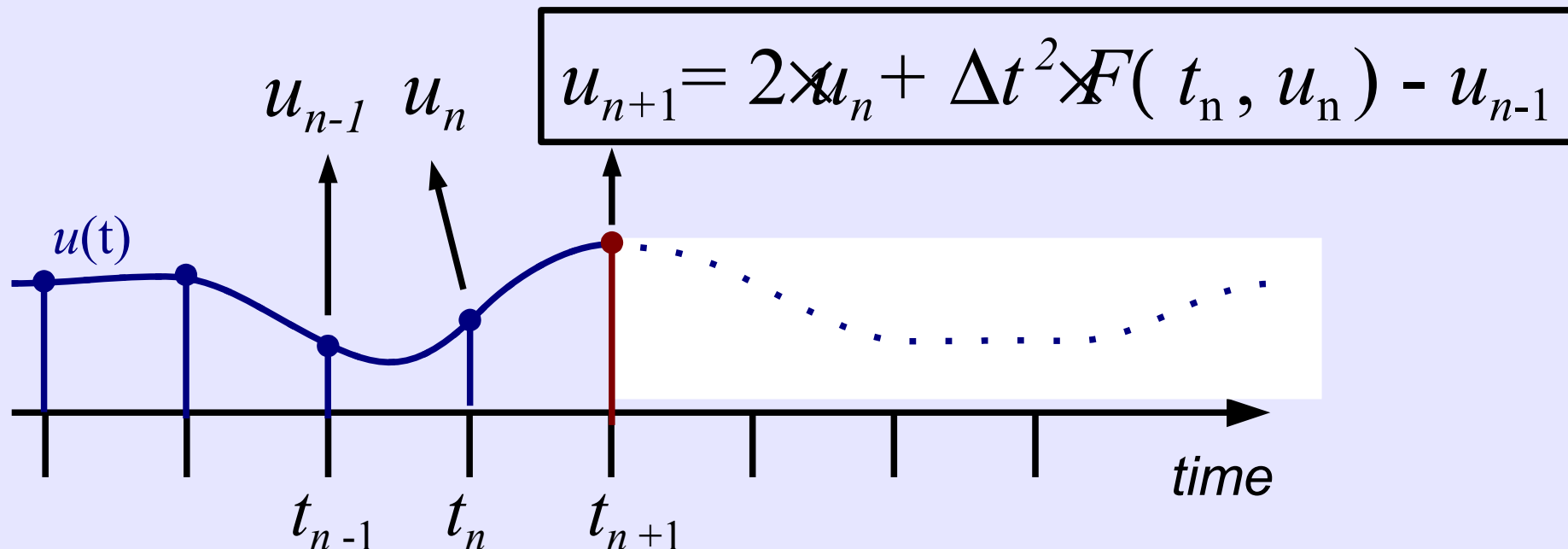


## Explicit two step time integration

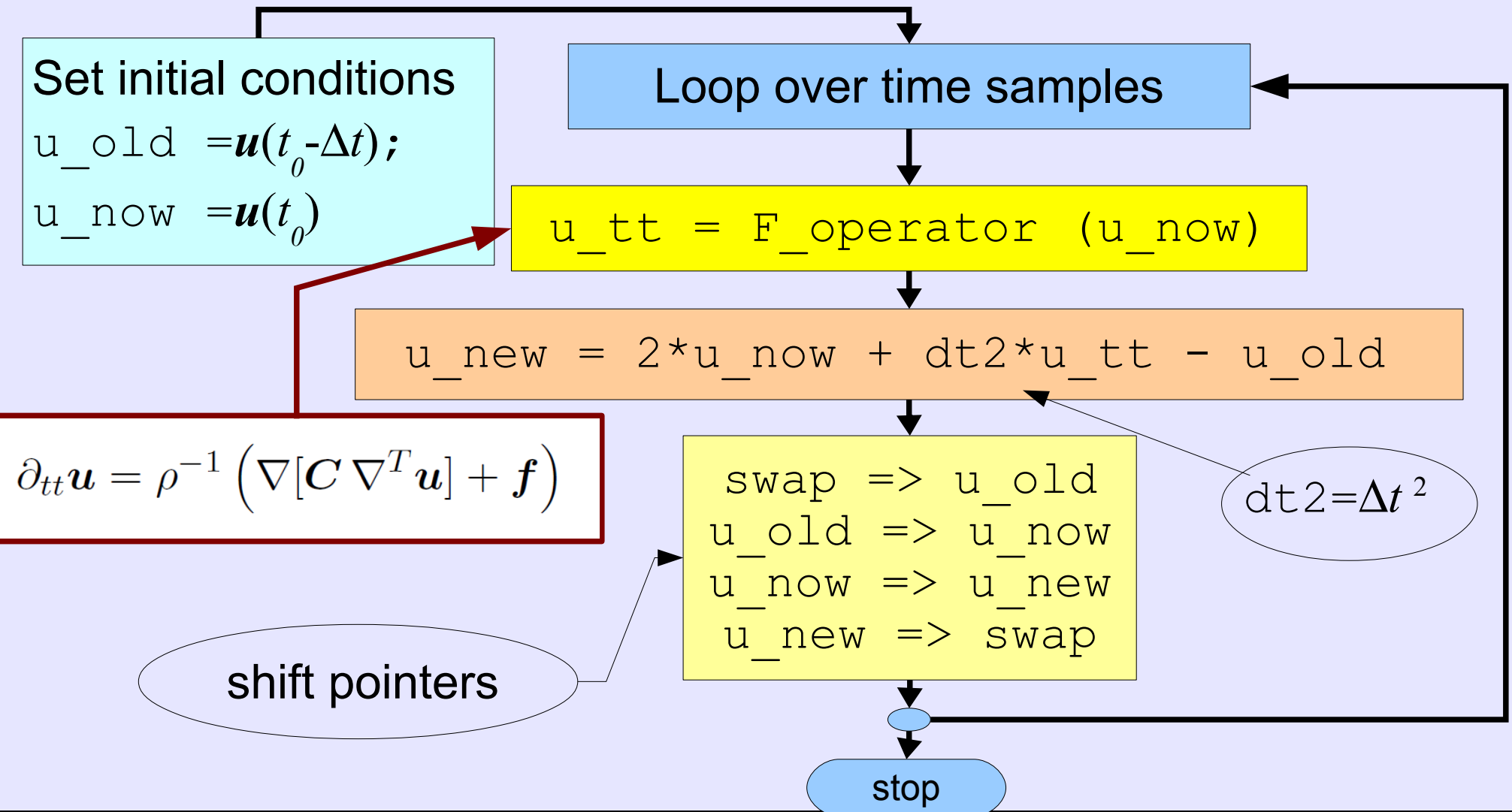
$$\begin{cases} \partial_{tt} \mathbf{u}(\mathbf{x}, t) = F(t, \mathbf{u}(\mathbf{x}, t)) \\ \mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0 \\ \mathbf{u}(\mathbf{x}, -\Delta t) = \mathbf{u}_{-1} \end{cases}$$

Discretization of the time axis

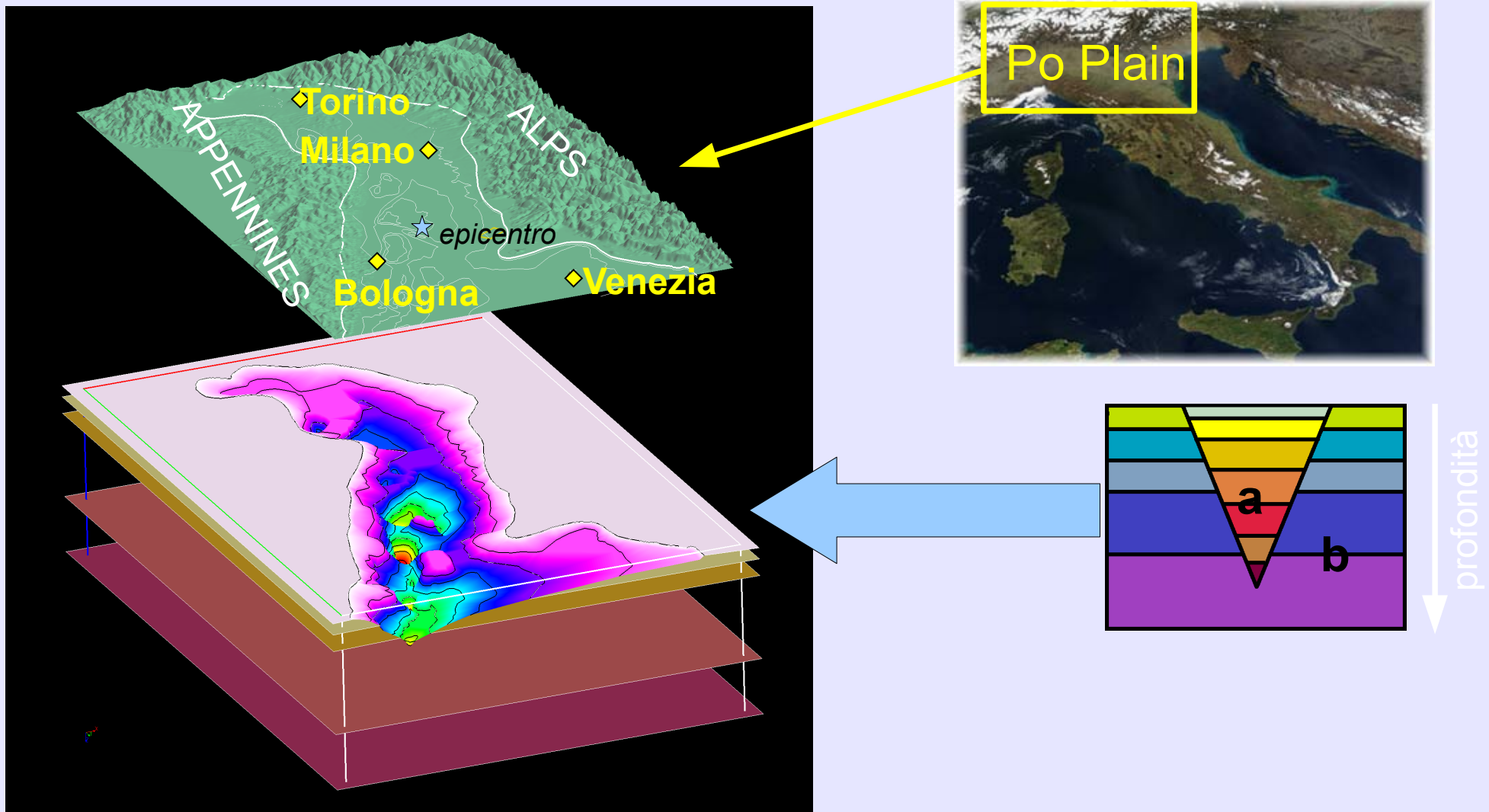
$$t_{n+1} = t_n + \Delta t \quad \forall n \in \{0, 1, \dots, N\}$$



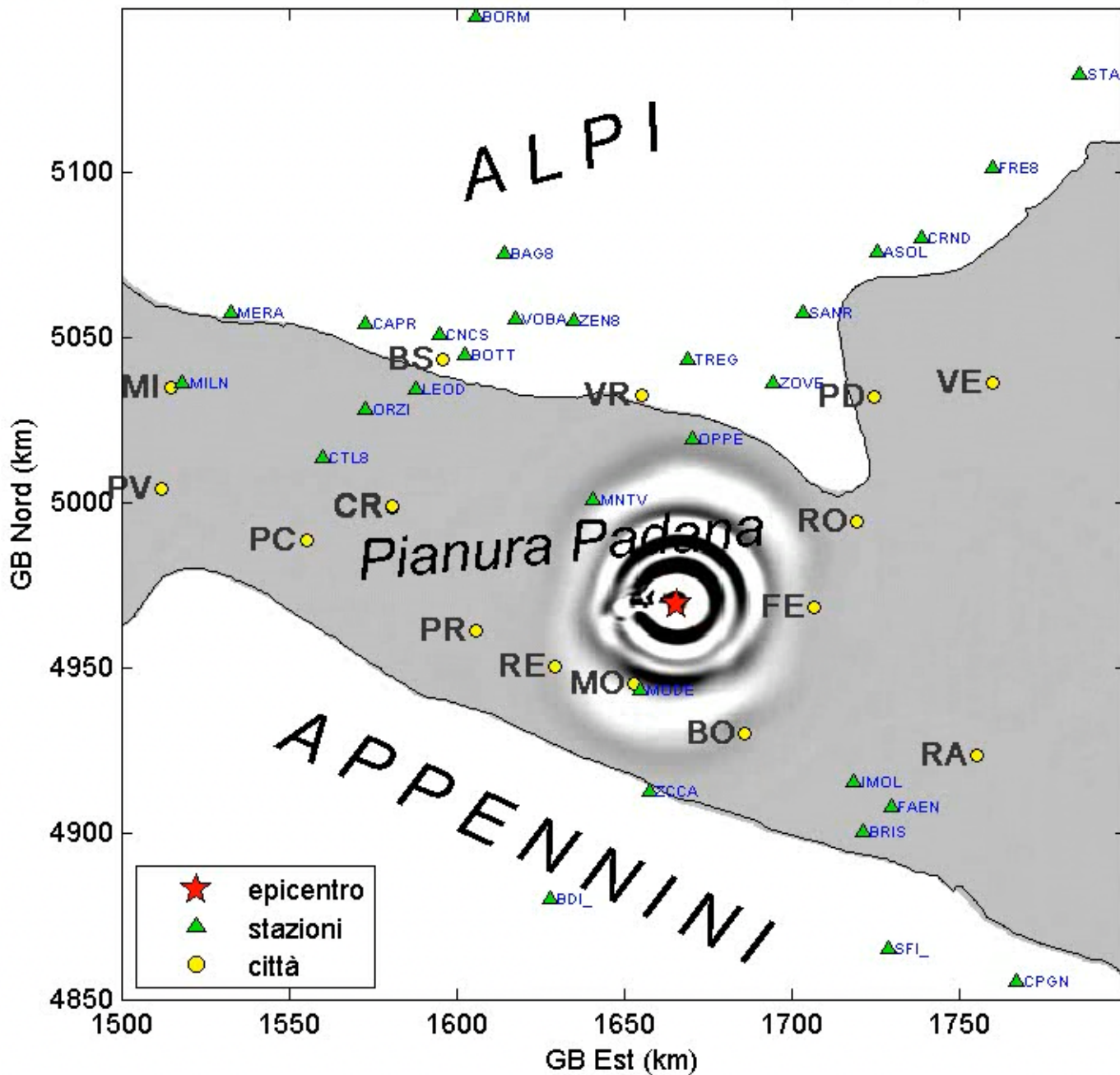
# Explicit two step time integration



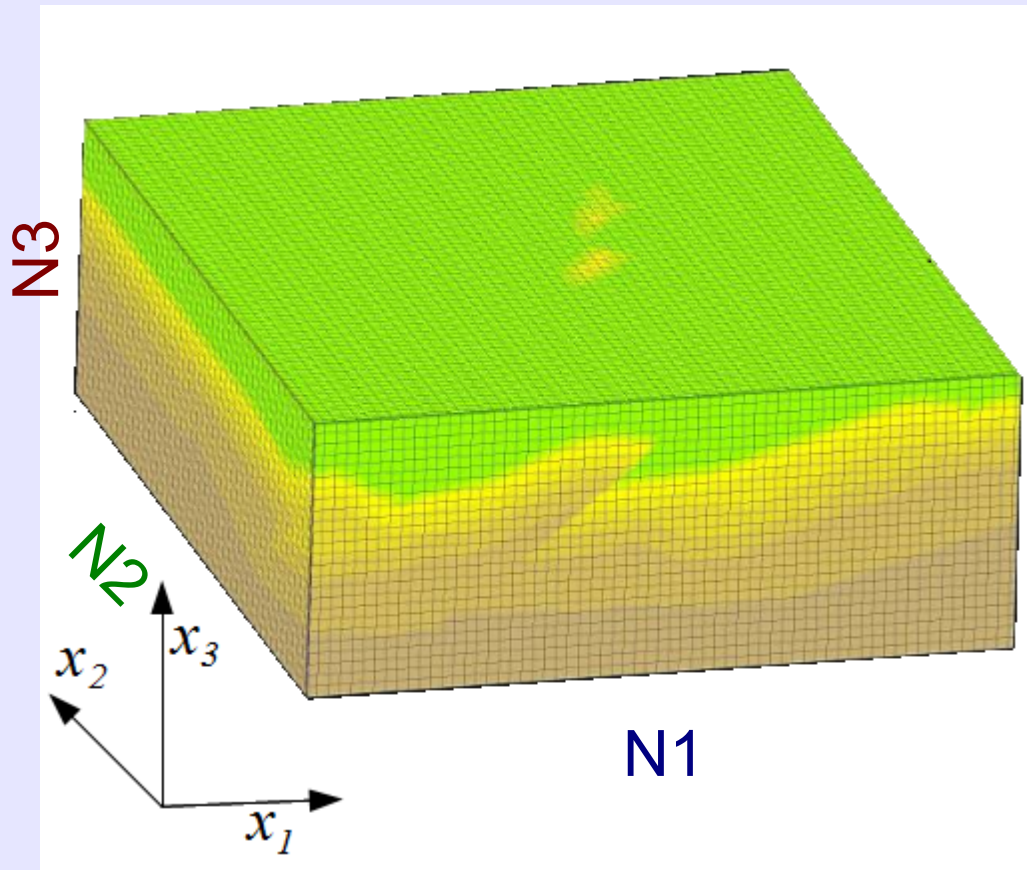
# Simulation of earthquake ground motion



Evento simulato: 2012-05-20 03:02:50 M=4.9 ; Tempo di propagazione: 12.5 s.



# Simulation of earthquake ground motion



Dimension of the problem (Po Plain):

$N1=768$ ;  $N2=768$ ;  $N3=192$ ;

$N=N1*N2*N3=1132462082$

$N \sim 2^{27}$

$N \sim 10^9$

$NT=60000=6*10^4$

Runtime:  $NT*6*N*(15+2*\log_2(N))$

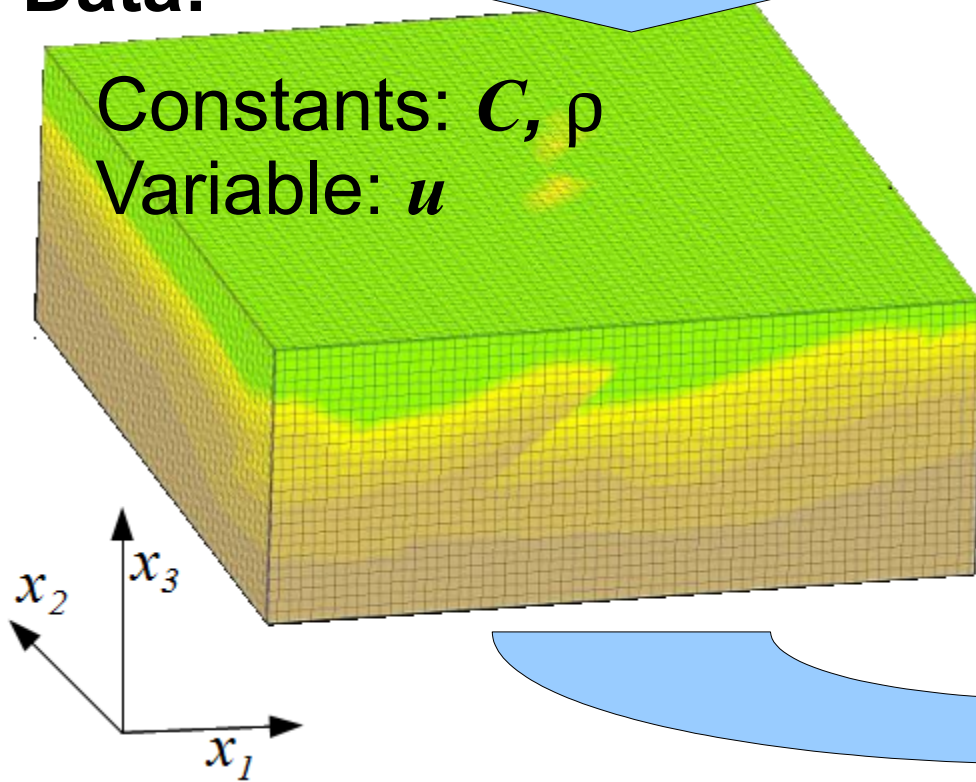
$\sim 2.5 * 10^{17}$



# Parallelization of the code

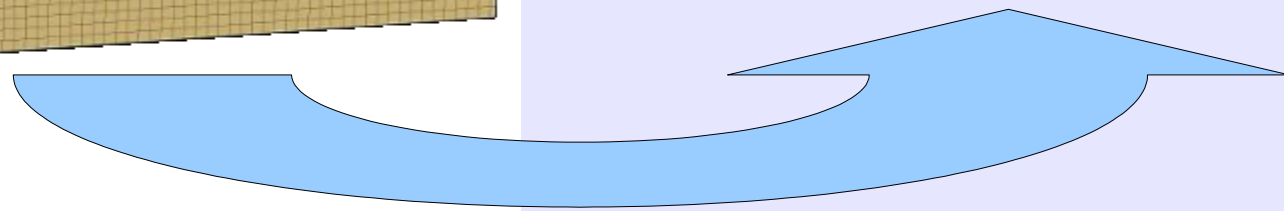
**Data:**

Constants:  $C, \rho$   
Variable:  $u$

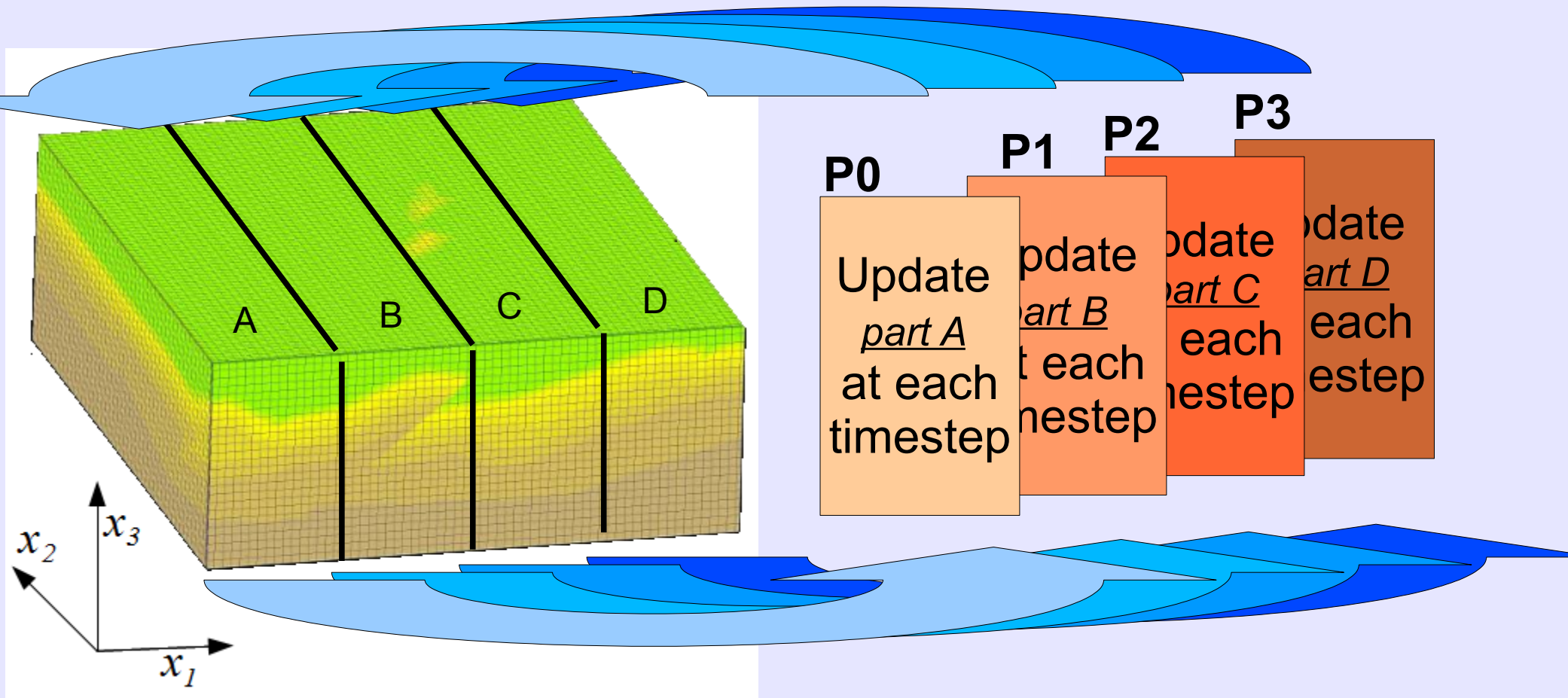


**Task:**

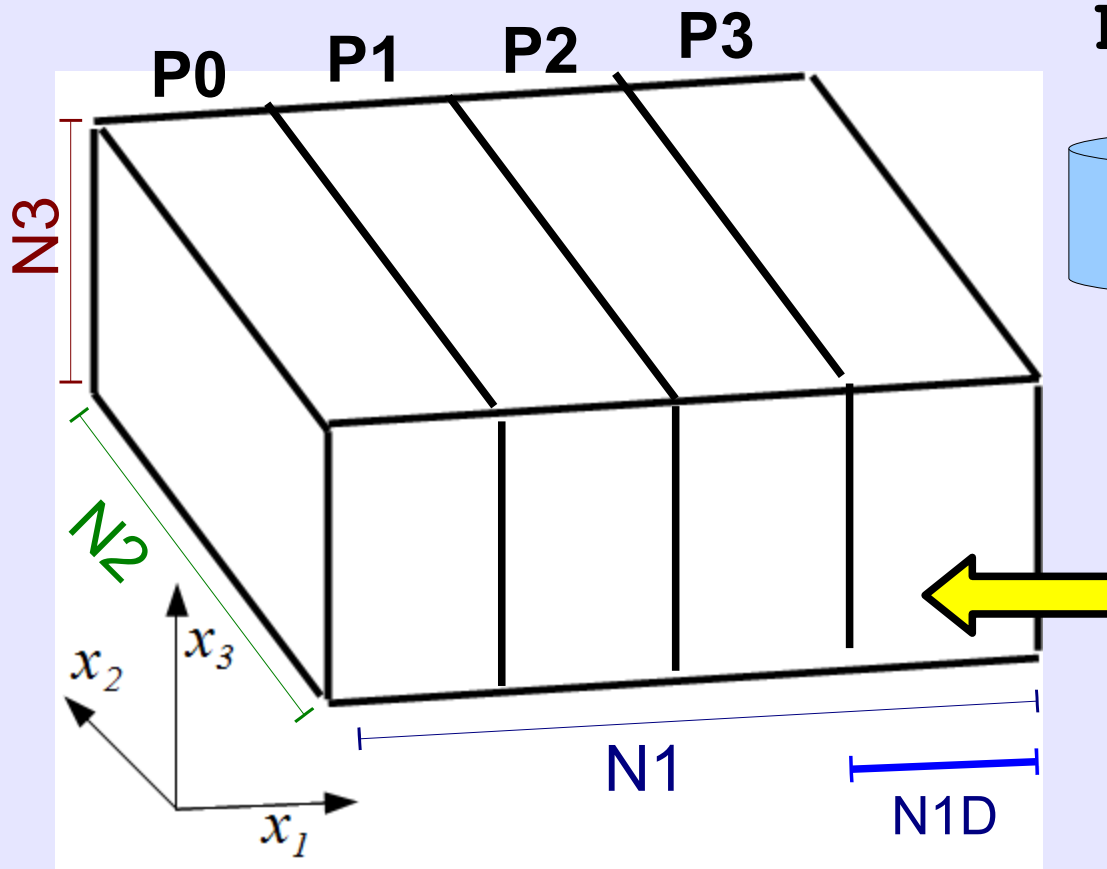
Update  $u$   
at each timestep



# Parallelization of the code



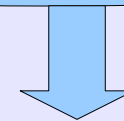
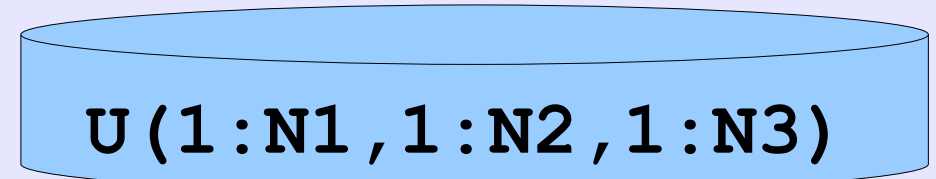
# 1D domain decomposition



$NP$  = number of processes

$N1D = N1 / NP$

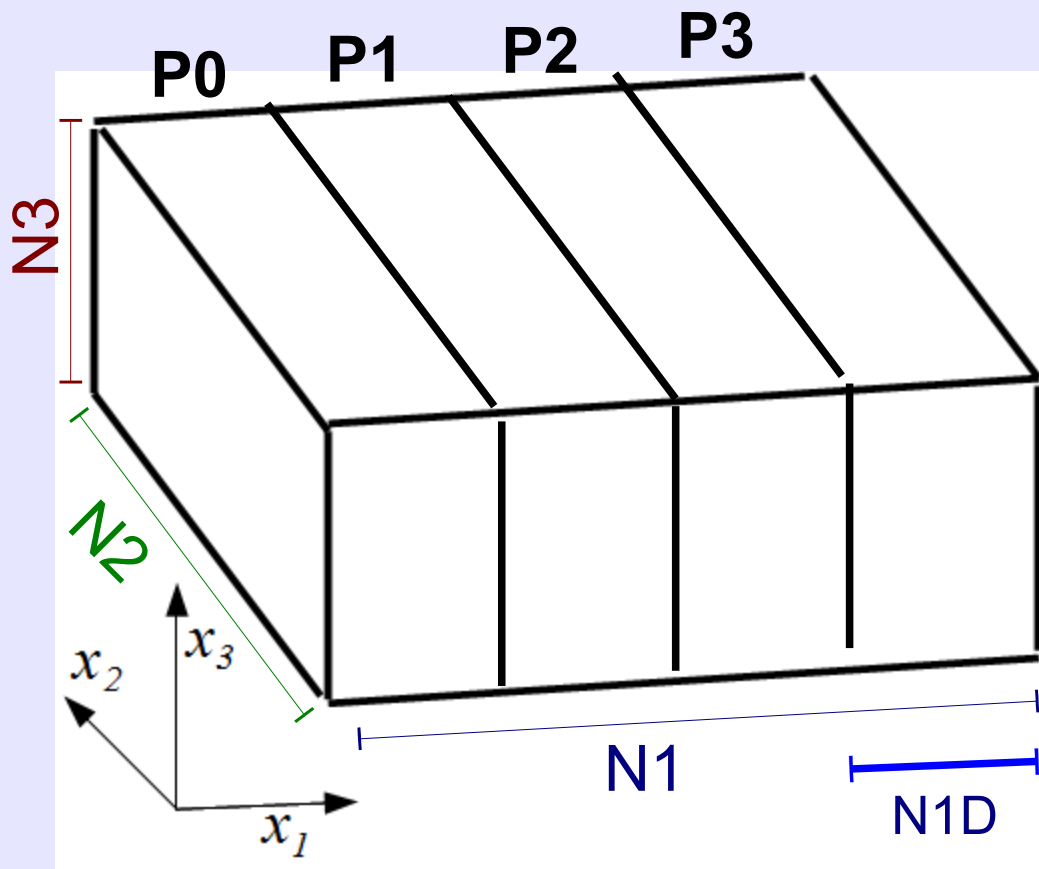
on disk



$U(1:N1D, 1:N2, 1:N3)$   
 $D1U(1:N1D, 1:N2, 1:N3)$   
 $D2U(1:N1D, 1:N2, 1:N3)$   
 $D3U(1:N1D, 1:N2, 1:N3)$

in each processor's ram

# 1D domain decomposition



$NP$  = number of processes

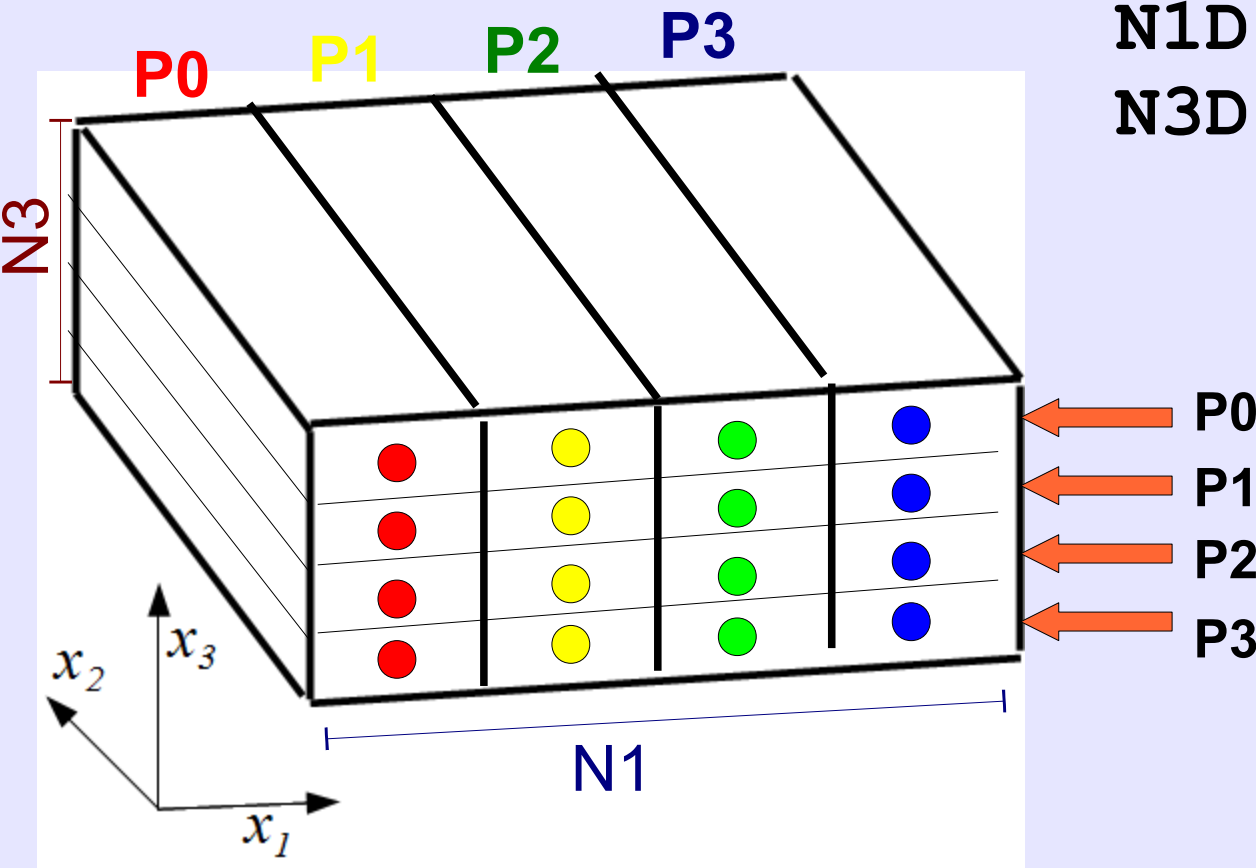
$N1D = N1 / NP$

$U(1 : N1D, 1 : N2, 1 : N3)$

$\partial_3$  &  $\partial_2$  embarrassingly parallel

$\partial_1$  needs communication!

# 1D domain decomposition

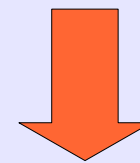


$NP$  = number of processes

$N1D = N1 / NP$

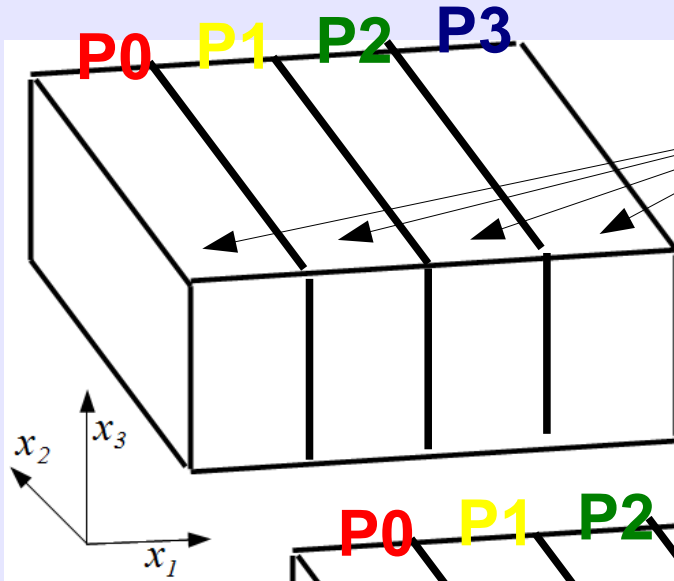
$N3D = N3 / NP$

$U(1:N1D, 1:N2, 1:N3)$   
suitable for  $\partial_3$  &  $\partial_2$



$U(1:N1, 1:N2, 1:N3D)$   
suitable for  $\partial_1$  (&  $\partial_2$ )

# 1D domain decomposition

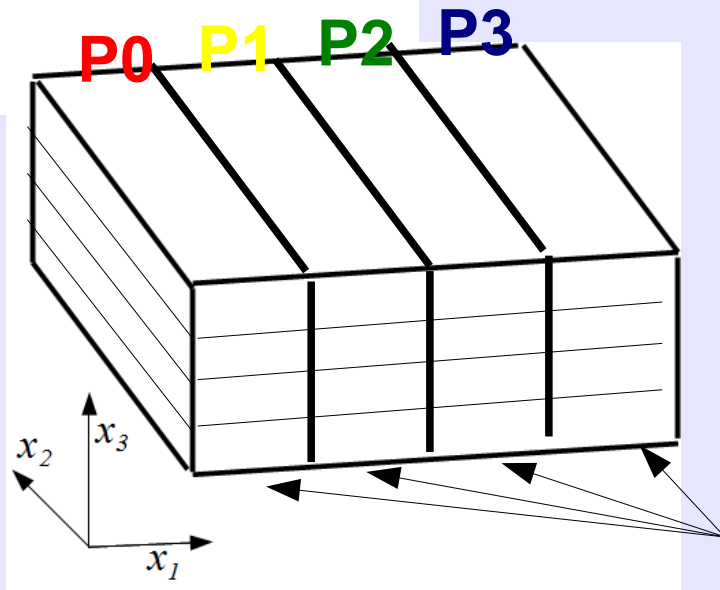


$U(1:N1D, 1:N2, 1:N3)$

$NP$  = number of processes

$N1D = N1/NP$

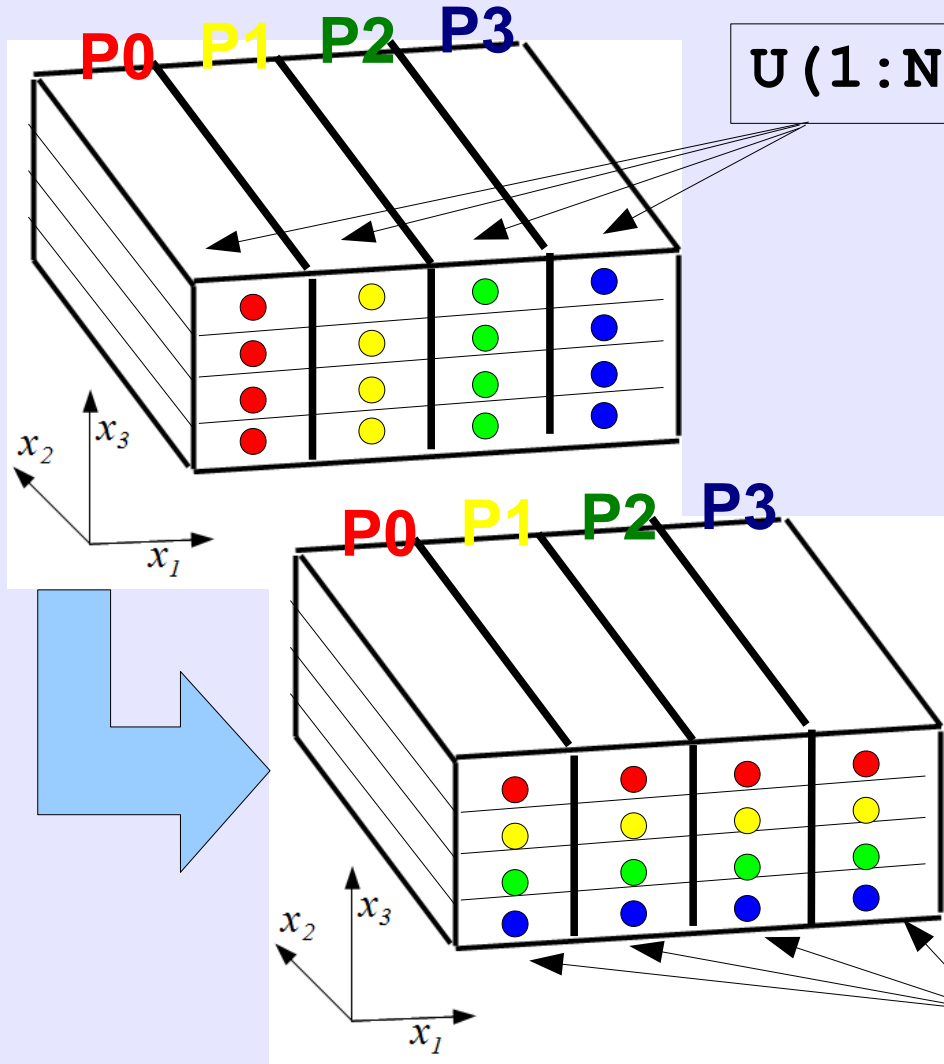
$N3D = N3/NP$



Container for data from other processes

$B(1:N1D, 1:N2, 1:N3D, 1:NP)$

# 1D domain decomposition



$U(1:N1D, 1:N2, 1:N3)$

NP = number of processes  
 $N1D = N1/NP$   
 $N3D = N3/NP$

```

INTEGER :: NB=N1D*N2*N3D
!FROM U TO B
CALL MPI_ALLTOALL&
      (U,NB,MPI_REAL,&
       B,NB,MPI_REAL,&
       MPI_COMM_WORLD,IERR)
  
```

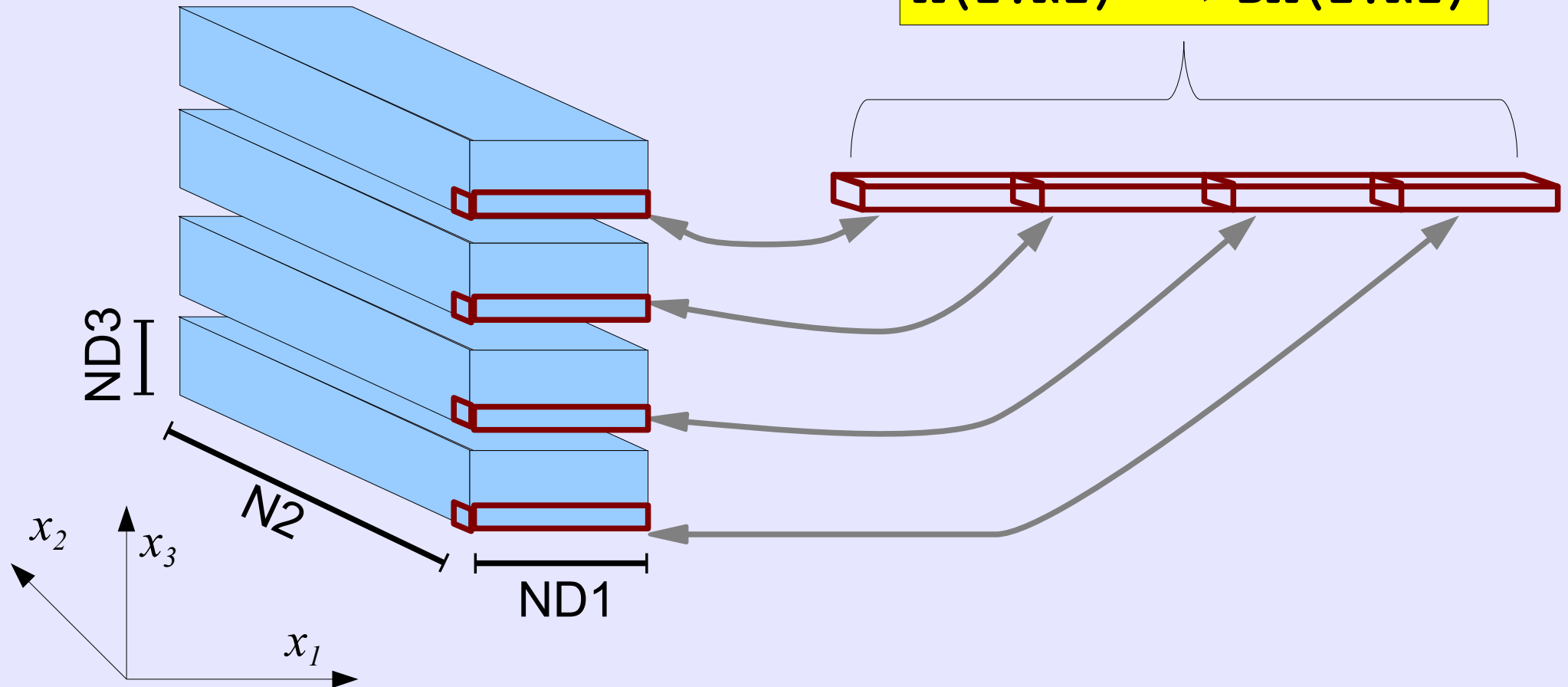
$B(1:N1D, 1:N2, 1:N3D, 1:NP)$

# 1D domain decomposition

$B(1:ND1, 1:N2, 1:ND3, 1:NP)$

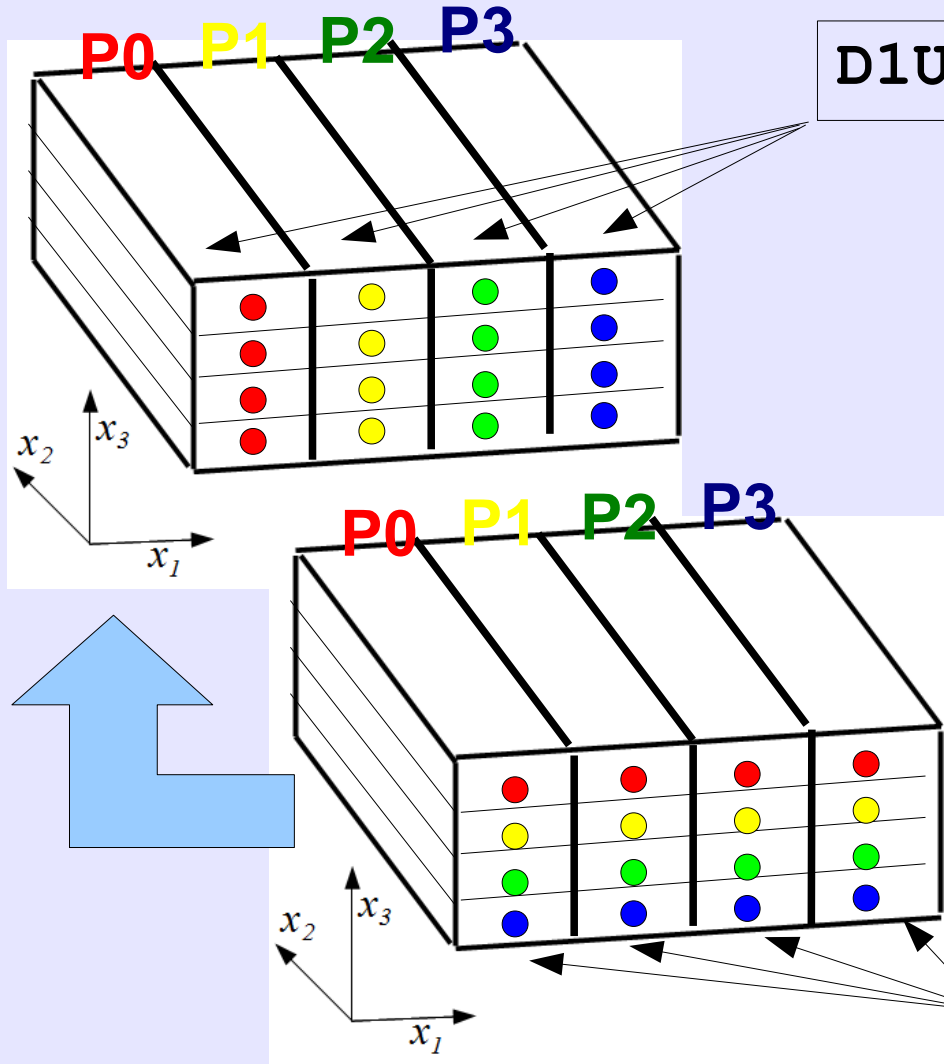
Perform derivative "à la Fourier"

$A(1:N1) \longrightarrow DA(1:N1)$





# 1D domain decomposition



`D1U (1:N1D, 1:N2, 1:N3)`

NP = number of processes  
 N1D = N1/NP  
 N3D = N3/NP

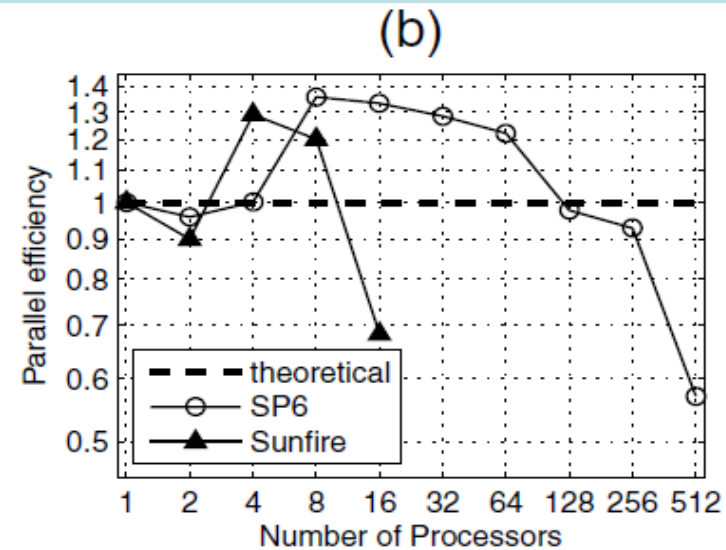
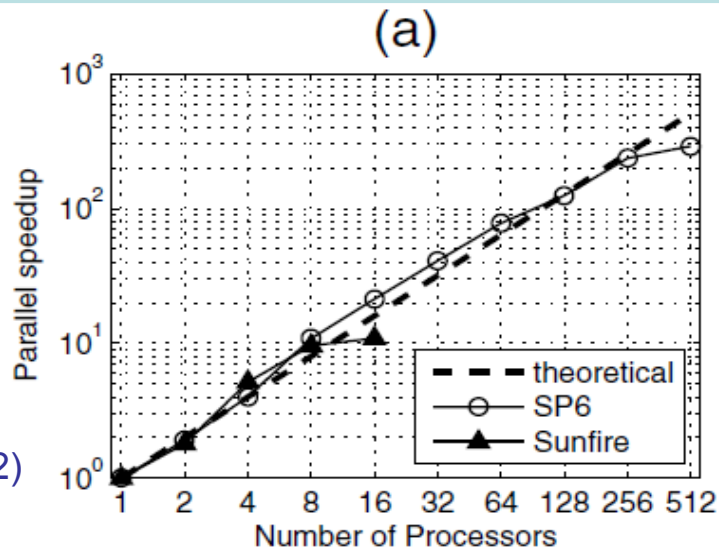
INTEGER :: NB=N1D\*N2\*N3D  
 !FROM U TO B

CALL MPI\_ALLTOALL&  
 (B,NB,MPI\_REAL,&  
 D1U,NB,MPI\_REAL,&  
 MPI\_COMM\_WORLD,IERR)

`B (1:N1D, 1:N2, 1:N3D, 1:NP)`

# Efficiency of 1D domain decomposition

strong  
scaling  
constant  
problem  
size  
(512 x 512 x 512)



## Limitations of the 1D domain decomposition:

- All processes communicate with all processes
- Number of processes  $\leq$  Number of samples along the shorter direction

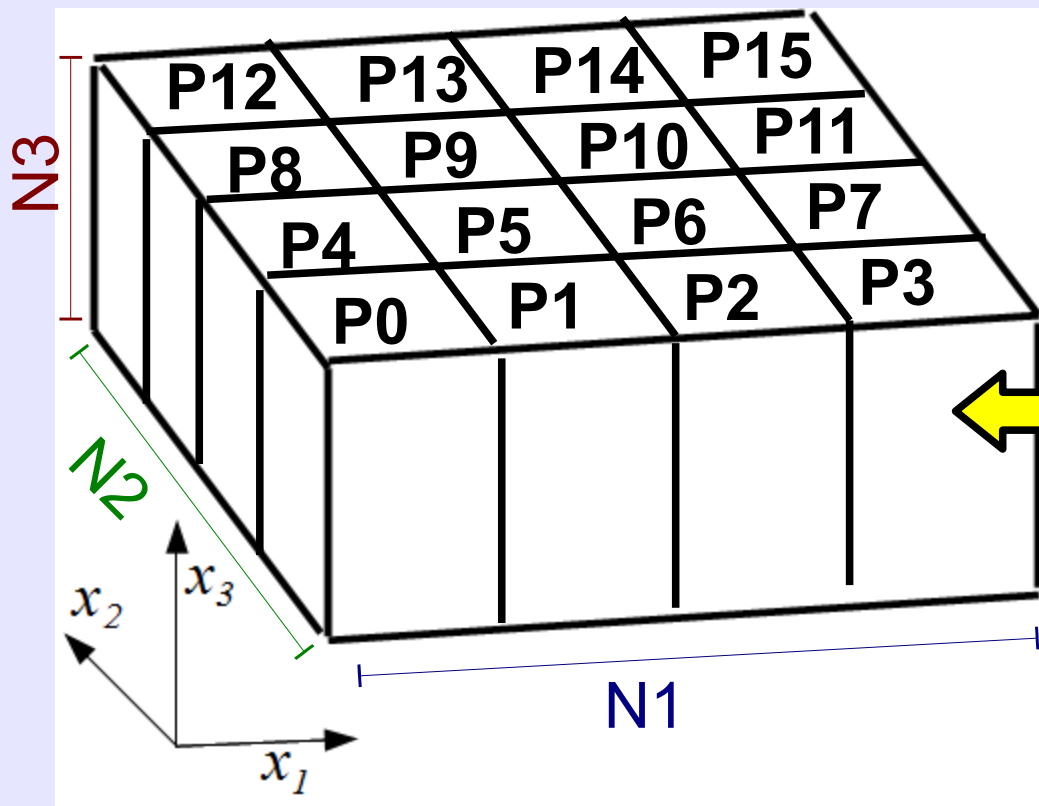
## 2D domain decomposition

number of processes:

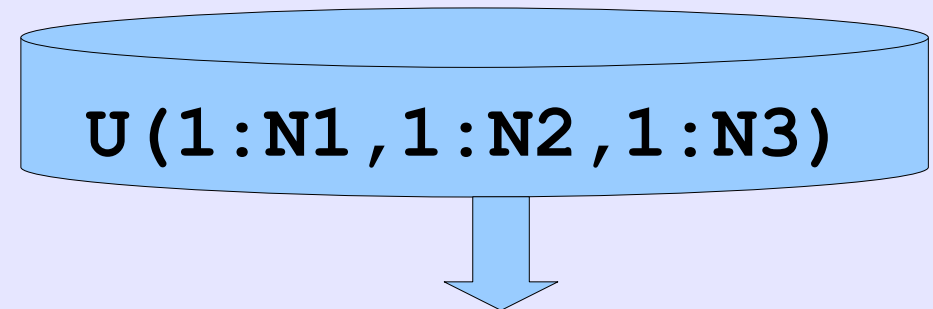
$$NP = NPS * NPS \quad !NPS > 0$$

$$N1D = N1 / NPS$$

$$N2D = N2 / NPS$$



on disk



$$U(1:N1, 1:N2, 1:N3)$$

$U(1:N1D, 1:N2D, 1:N3)$   
in each processor's ram

$\partial_3$  embarrassingly parallel

$\partial_1$  &  $\partial_2$  need communication!

## 2D domain decomposition

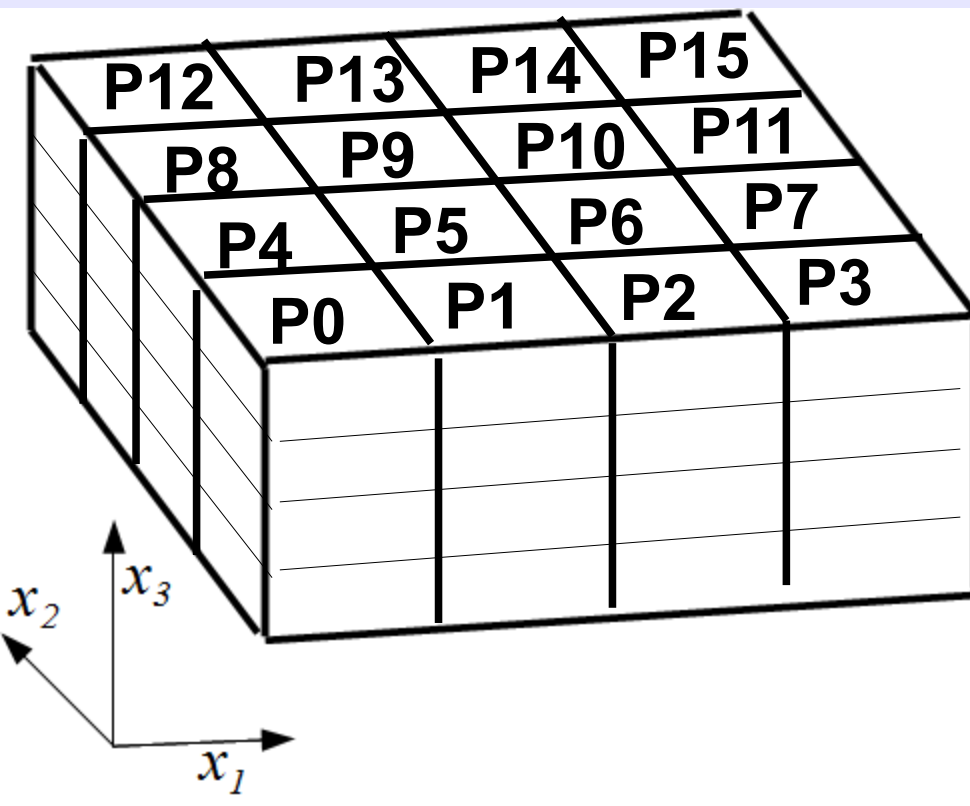
number of processes:

$$NP = NPS * NPS \quad !NPS > 0$$

$$N1D = N1 / NPS$$

$$N2D = N2 / NPS$$

$$N3D = N3 / NPS$$



$U(1:N1D, 1:N2D, 1:N3)$

$B(1:N1D, 1:N2D, 1:N3D, 1:NPS)$

Container for data from other processes

## 2D domain decomposition

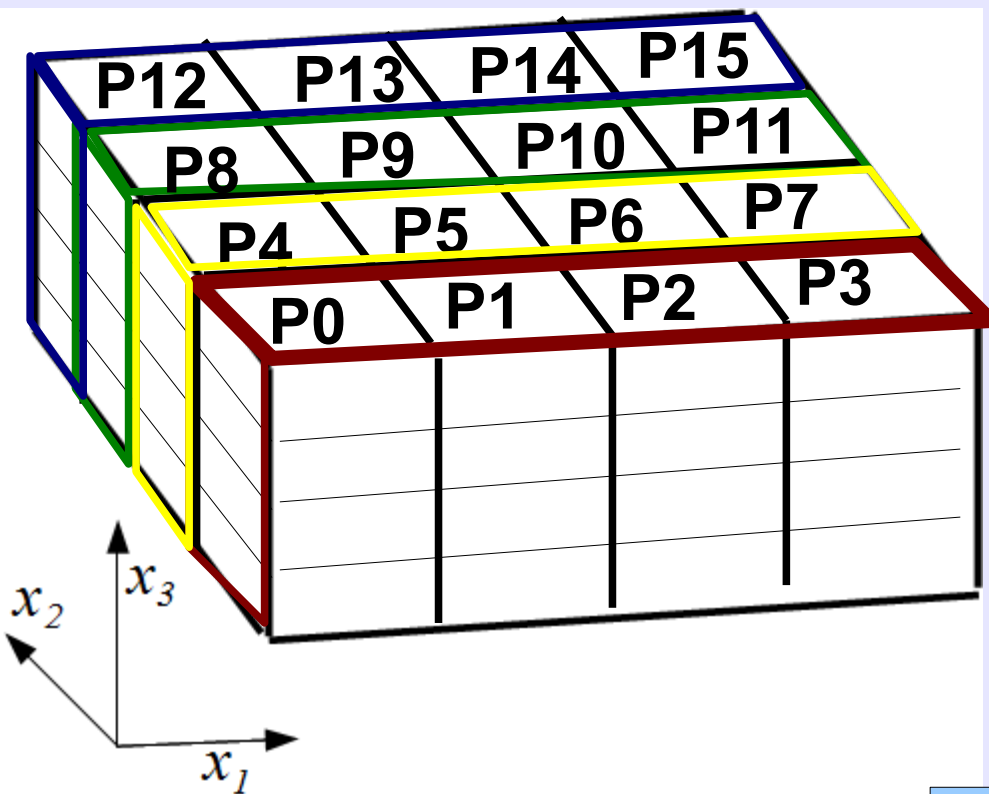
number of processes:

$$NP = NPS * NPS \quad !NPS > 0$$

$$N1D = N1 / NPS$$

$$N2D = N2 / NPS$$

$$N3D = N3 / NPS$$



```
U (1:N1D, 1:N2D, 1:N3)
```

```
B (1:N1D, 1:N2D, 1:N3D, 1:NPS)
```

```
INTEGER :: NB=N1D*N2*N3D
```

```
!FROM U TO B ONLY FOR D1
```

```
CALL MPI_ALLTOALL&
```

```
(U, NB, MPI_REAL, &
```

```
B, NB, MPI_REAL, &
```

```
COMM1, IERR)
```

MPI\_COMM\_WORLD

DIFFERS!

## 2D domain decomposition

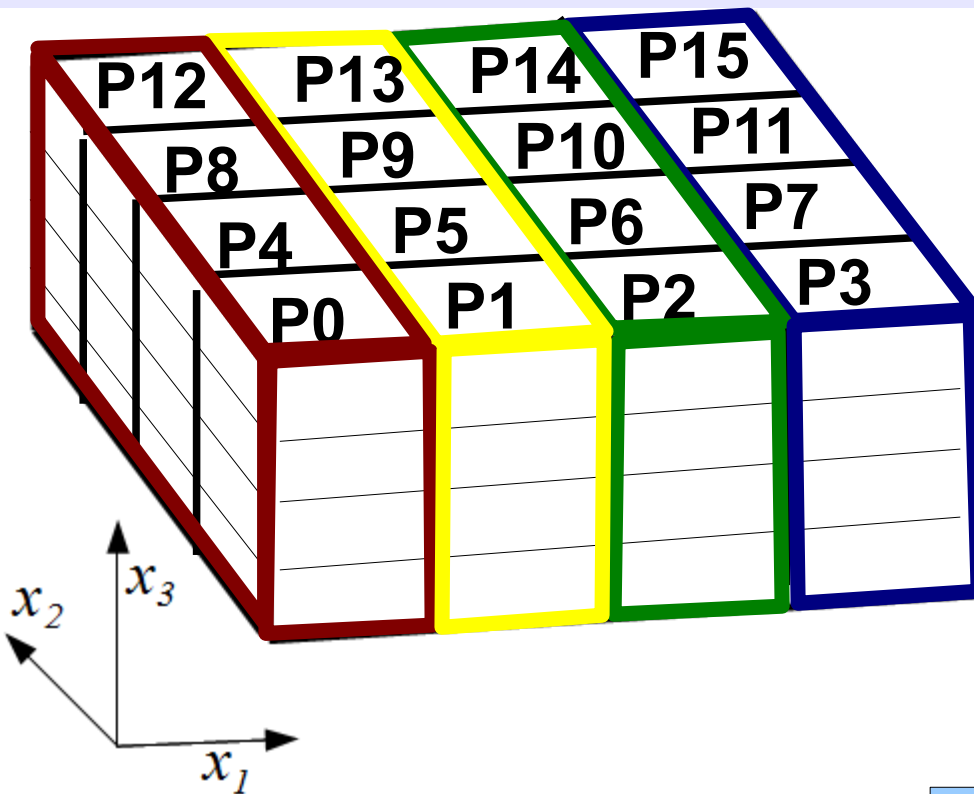
number of processes:

$$NP = NPS * NPS \quad !NPS > 0$$

$$N1D = N1 / NPS$$

$$N2D = N2 / NPS$$

$$N3D = N3 / NPS$$



$U(1:N1D, 1:N2D, 1:N3)$

$B(1:N1D, 1:N2D, 1:N3D, 1:NPS)$

INTEGER :: NB=N1D\*N2\*N3D

**!FROM U TO B ONLY FOR D2**

**CALL MPI\_ALLTOALL&**

**(U, NB, MPI\_REAL, &**

**B, NB, MPI\_REAL, &**

**COMM2, IERR)**

MPI\_COMM\_WORLD

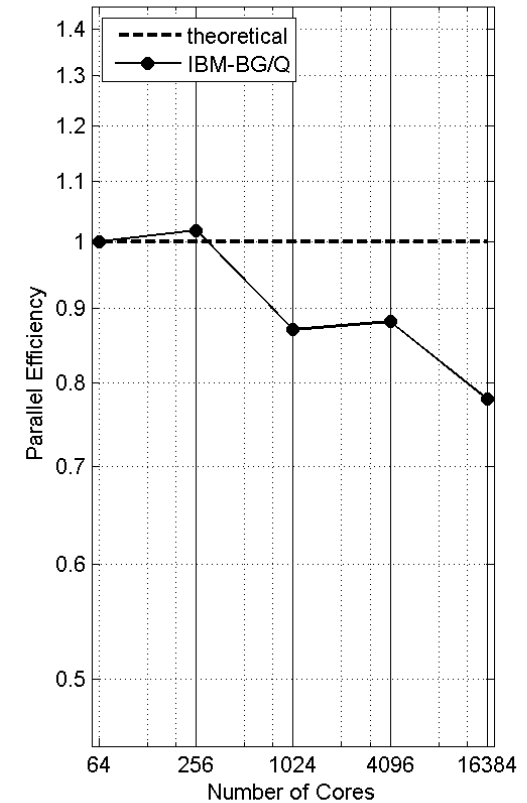
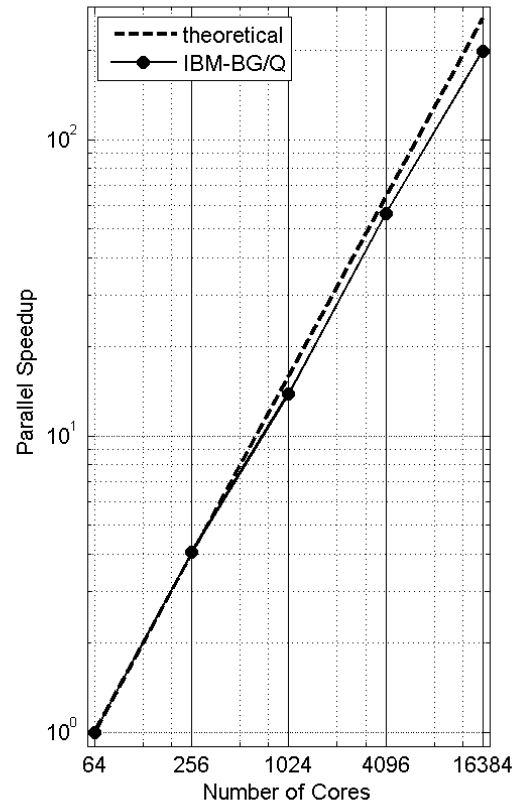
**DIFFERS!**

# Efficiency of 2D domain decomposition



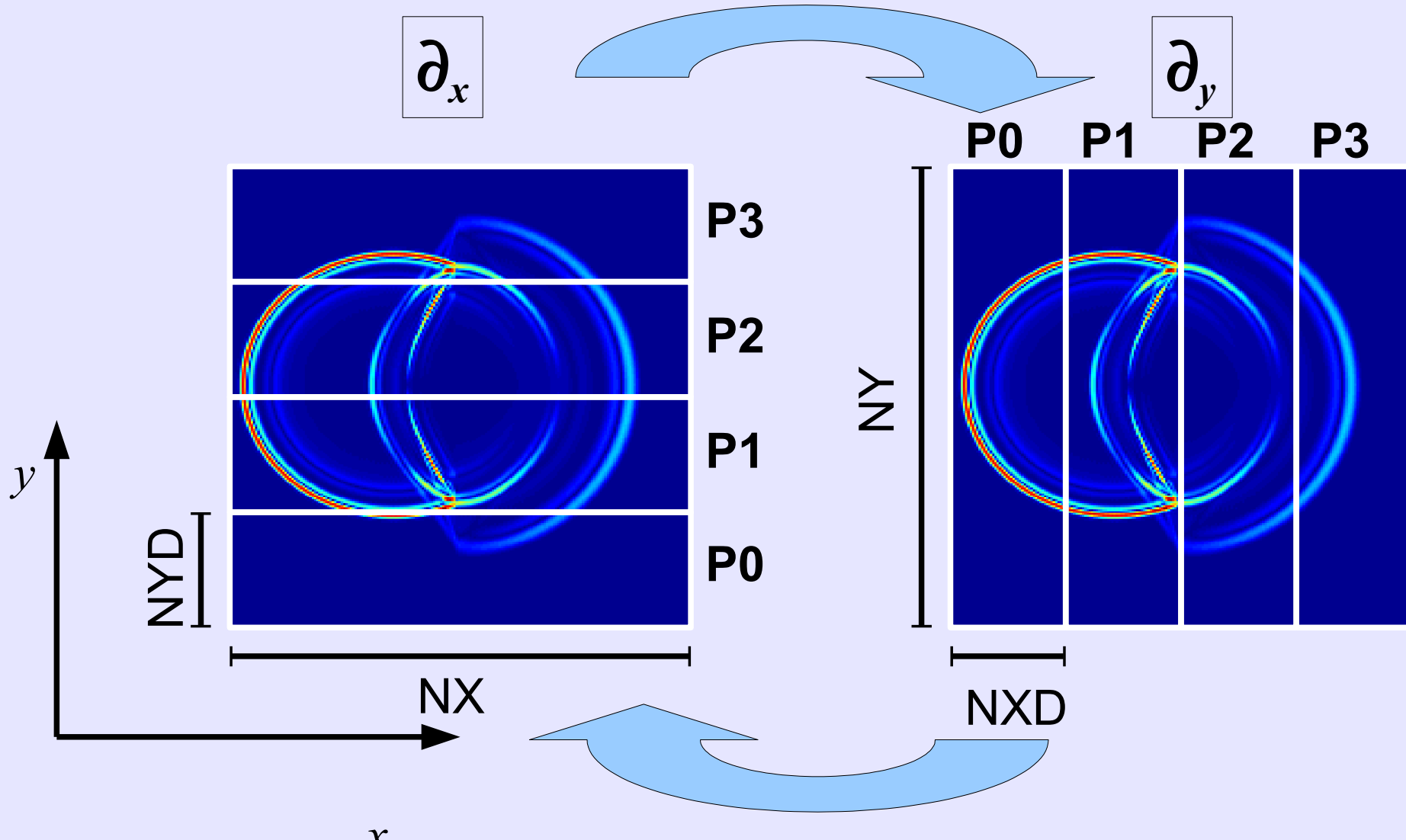
IBM BG/Q at CINECA

Strong scaling  
constant  
problem size  
(2048 x 2048 x 512)



2D domain decomposition allows to run FPSM  
on massively parallel computers!

# Lab-Session: implementing 2D wave simulation with MPI

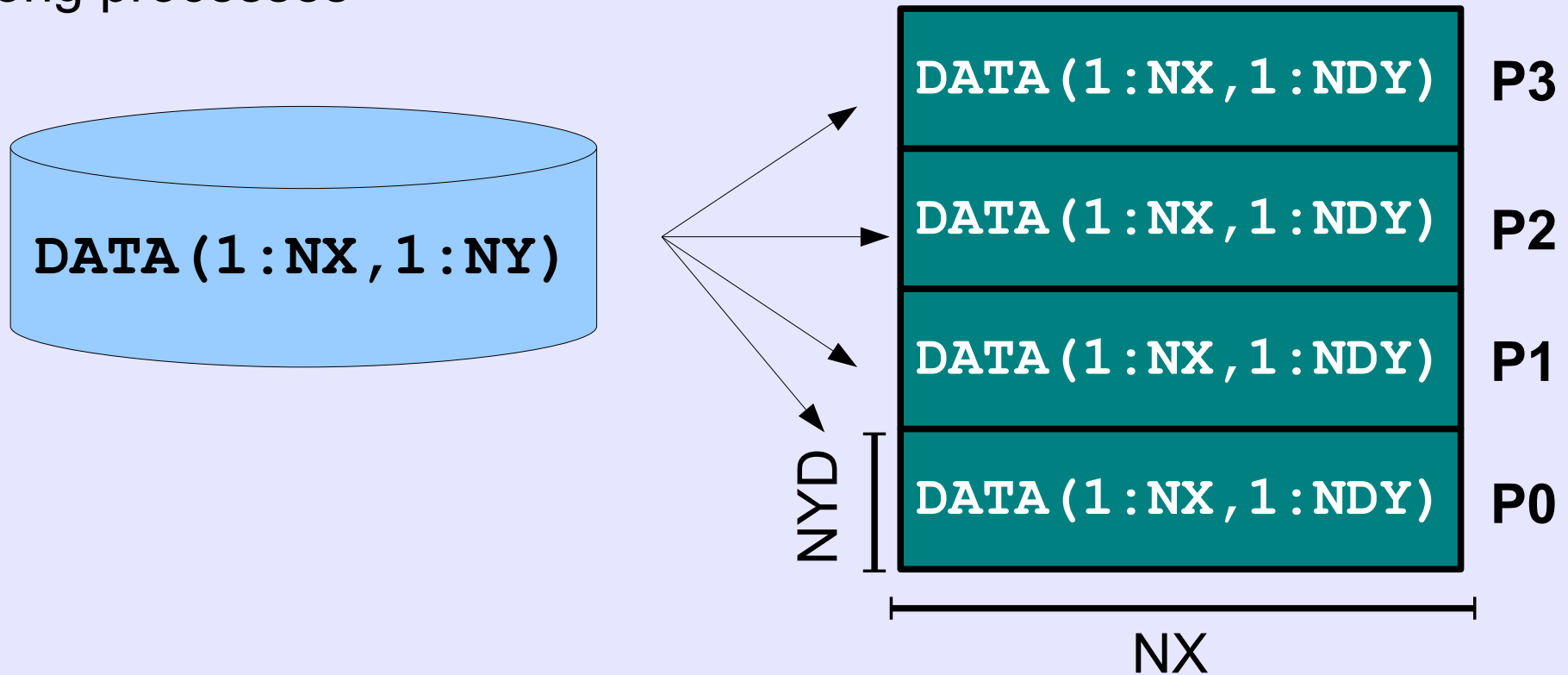




# Lab-Session: implementing 2D wave simulation with MPI

## Exercise 1: Space domain partitioning

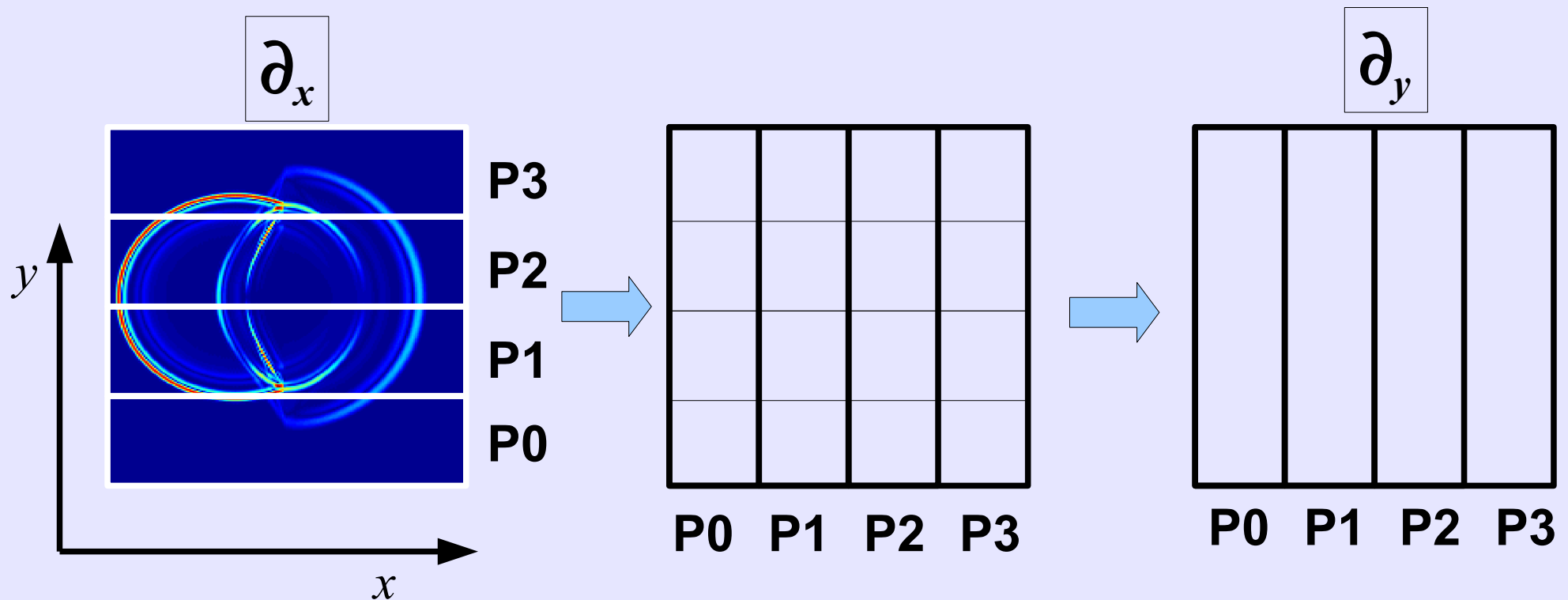
distribute input data (elastic parameters, initial values for  $u$ ) among processes



# Lab-Session: implementing 2D wave simulation with MPI

## Exercise 2: Partitioning rearrangement

Rearrange partitioning from  $\partial_x$  to  $\partial_y$  configuration





Thank you!

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