Particle-in-cell simulations

Part III: Boundary conditions and parallelization

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Plan of the lectures

- **Wednesday:**

  - *Morning:* The PIC method, numerical schemes and main algorithms.

  - *Afternoon:* Coding practice of the Boris push and the Yee algorithm.

- **Thursday:**

  - *Morning:* Implementation of Zeltron, structure and methods.

  - *Afternoon:* Zeltron hands on relativistic reconnection simulations

  - *Evening*: Seminar applications of PIC to relativistic magnetospheres.

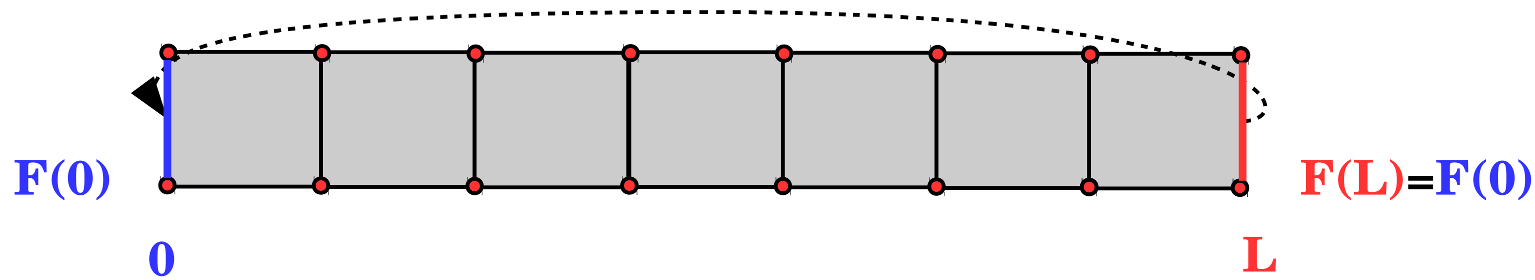
- ***Friday:***

  - *Morning: B*oundary conditions and parallelization in Zeltron.

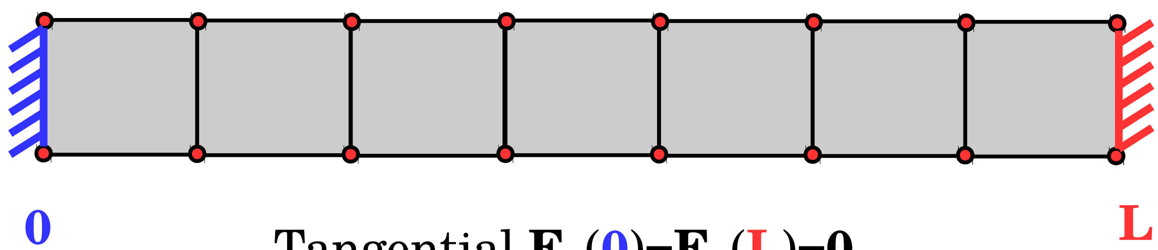
  - *Afternoon:* Zeltron Hands on relativistic collisionless shocks simulations

Field boundary conditions: a few examples

Periodic



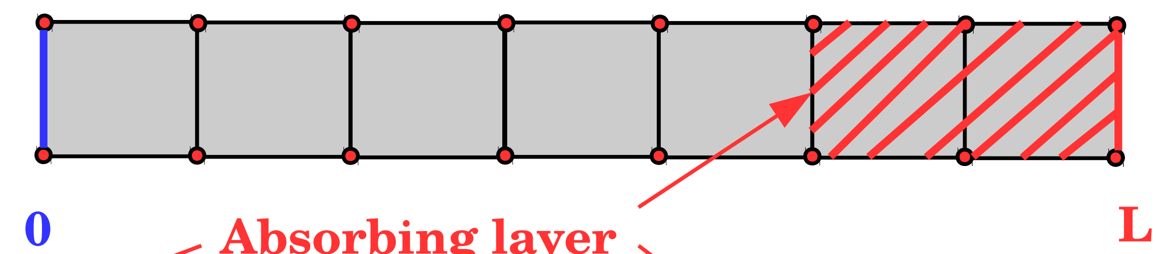
Perfectly conducting walls



Tangential $\mathbf{E}_T(0)=\mathbf{E}_T(L)=0$

Perpendicular $\mathbf{B}_\perp(0)=\mathbf{B}_\perp(L)=0$

Absorbing layer (open boundary)



Absorbing layer

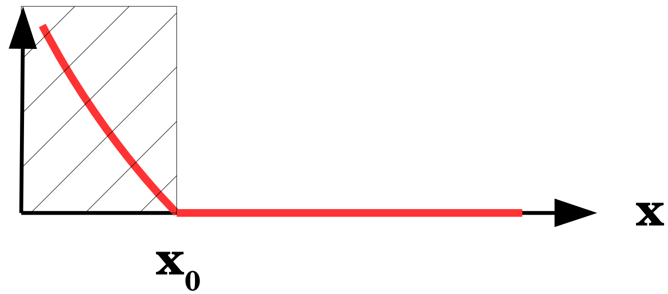
$$\frac{\partial \boldsymbol{E}}{\partial t}+\sigma \boldsymbol{E}=c\nabla\times\boldsymbol{B}-4\pi\boldsymbol{J} \qquad \frac{\partial \boldsymbol{B}}{\partial t}+\sigma^*\boldsymbol{B}=-c\nabla\times\boldsymbol{E}$$

Example of a 1D absorbing layer

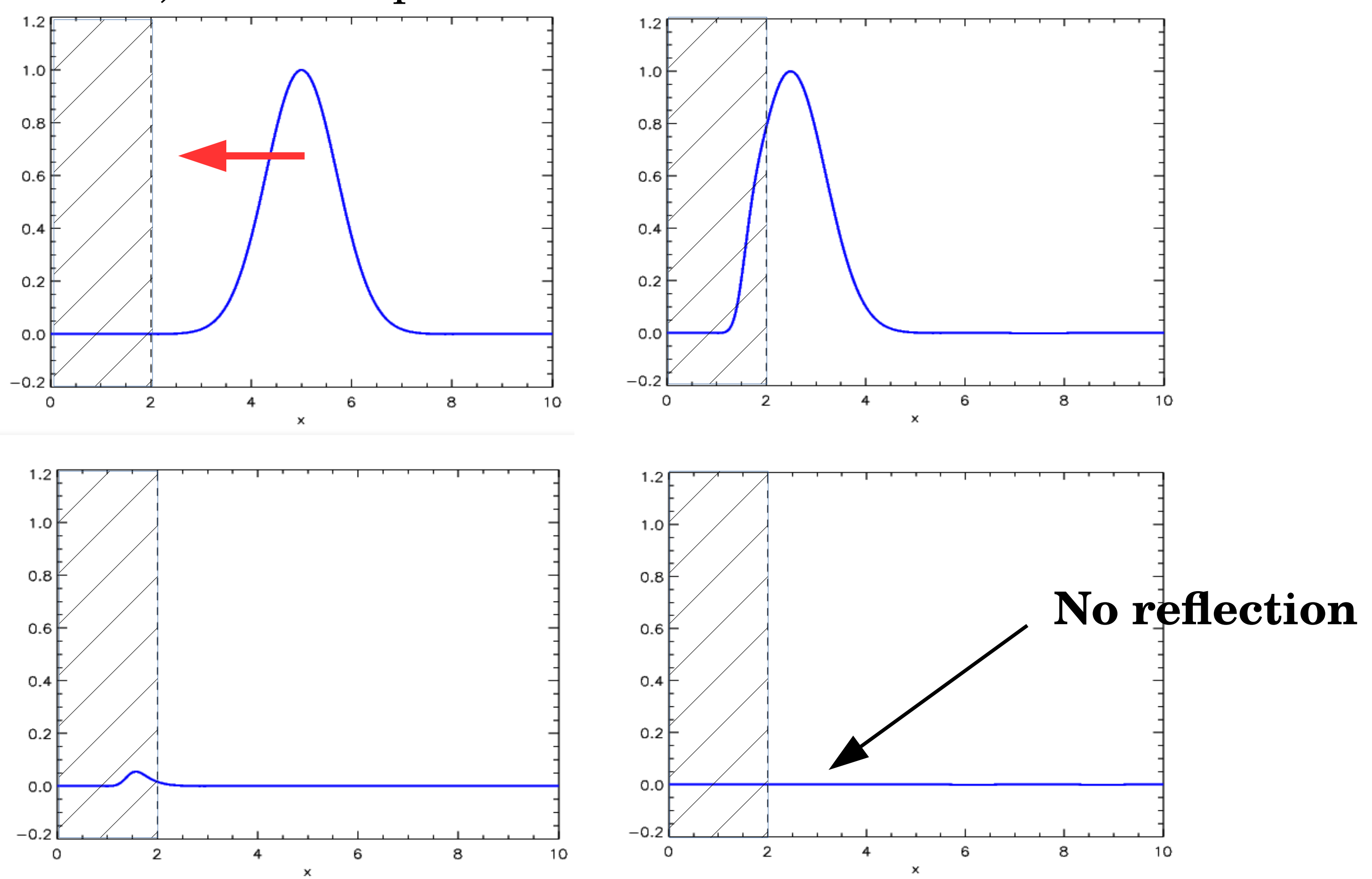
Absorption without reflection => **Gradially increasing** conductivity

For example :

$$\sigma = -\sigma_0 (x - x_0)^3$$



t=0, Gaussian pulse



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Perfectly Matched Layer (PML)

$$\frac{\partial \boldsymbol{E}}{\partial t}+\sigma \boldsymbol{E}=c\nabla\times\boldsymbol{B}-4\pi\boldsymbol{J} \qquad \frac{\partial \boldsymbol{B}}{\partial t}+\sigma^{*}\boldsymbol{B}=-c\nabla\times\boldsymbol{E}$$

Multi-D generalization : **Perfectly Matched Layer** (see *Bérenger 1994-1996*)

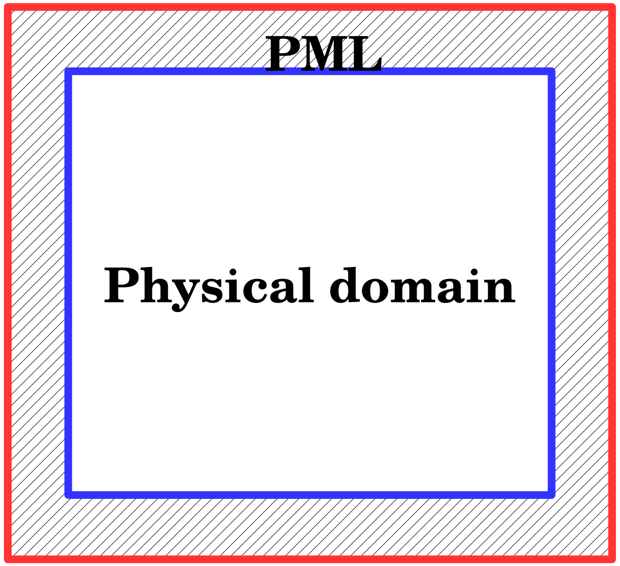
Example: Let's consider a 2D case in vacuum with E_x, E_y, and B_z.

Then, we have to solve these :

$$\frac{\partial E_y}{\partial t}=-c\frac{\partial B_z}{\partial x}$$ ⟶ **Wave along x**

$$\frac{\partial E_x}{\partial t}=c\frac{\partial B_z}{\partial y}$$ ⟶ **Wave along y**

$$\frac{\partial B_z}{\partial t}=-c\left(\frac{\partial E_y}{\partial x}-\frac{\partial E_x}{\partial y}\right)$$ ⟶ **Wave along x and y**



The trick is to split the B_z component into two : $B_z=B_{zx}+B_{zy}$

$$\frac{\partial E_y}{\partial t}+\sigma_x E_y=-c\frac{\partial}{\partial x}\left(B_{zx}+B_{zy}\right) \qquad \frac{\partial B_{zx}}{\partial t}+\sigma_x B_{zx}=-c\frac{\partial E_y}{\partial x}$$

$$\frac{\partial E_x}{\partial t}+\sigma_y E_x=c\frac{\partial}{\partial y}\left(B_{zx}+B_{zy}\right) \qquad \frac{\partial B_{zy}}{\partial t}+\sigma_y B_{zy}=c\frac{\partial E_x}{\partial y}$$

Easily generalized to all components in 2D and 3D.

Problem : 2 times more equations to solve !

Field boundary conditions in Zeltron

Choice of boundary conditions (mod_input.f90)

```
! Specify the boundary conditions for the fields:
! 1. "PERIODIC": Periodic boundary conditions
! 2. "METAL": Perfect metal with infinite conductivity

CHARACTER(LEN=10), PARAMETER, PUBLIC :: BOUND_FIELD_XMIN="PERIODIC"
CHARACTER(LEN=10), PARAMETER, PUBLIC :: BOUND_FIELD_XMAX="PERIODIC"
CHARACTER(LEN=10), PARAMETER, PUBLIC :: BOUND_FIELD_YMIN="PERIODIC"
CHARACTER(LEN=10), PARAMETER, PUBLIC :: BOUND_FIELD_YMAX="PERIODIC"
```

Perfectly conducting wall along x-direction for E_z (mod_fields.f90)

```
!***********************************************************************
! Check boundary conditions along X

IF (xminp.EQ.xmin) THEN

   IF (BOUND_FIELD_XMIN.EQ."METAL") THEN
   ! Tangent to conductor surface
   Ez(1,:)=0.0
   END IF

END IF

!***********************************************************************
```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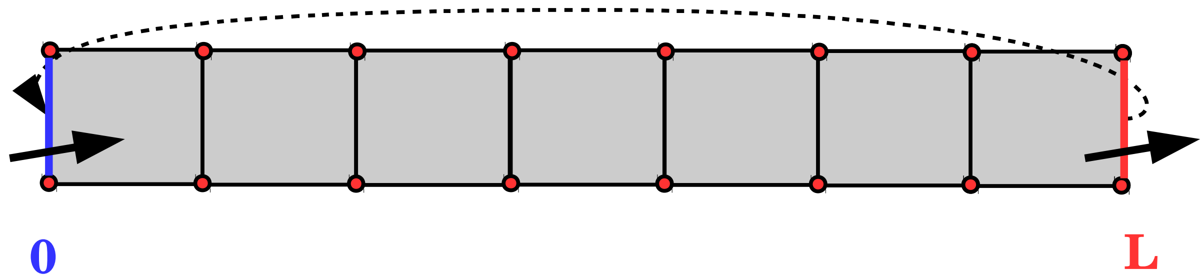
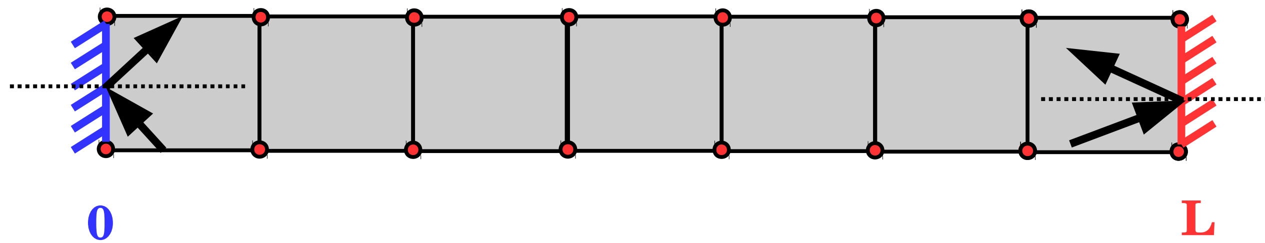
Particle boundary conditions: a few examples

Periodic

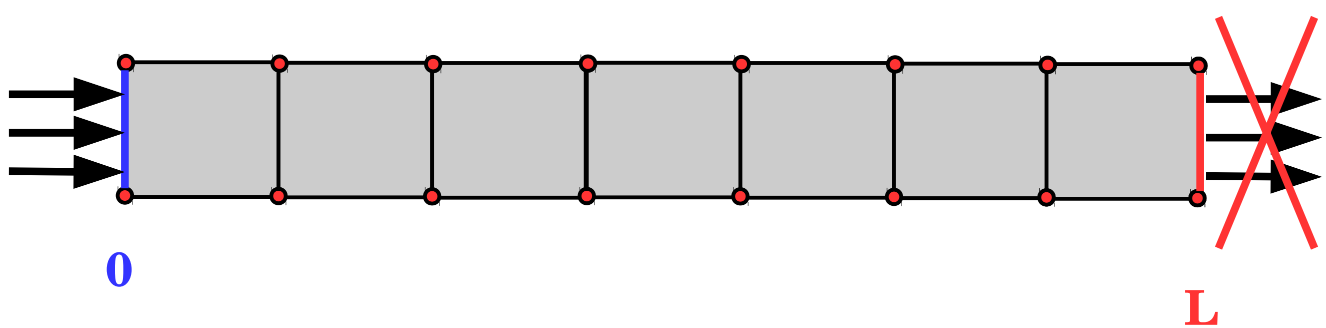


Perfectly reflective walls



Ex : At **x=L** **Positions :** $x \leftarrow 2L - x$, $y \leftarrow y$ **Velocities :** $v_x \leftarrow -v_x$, $v_y \leftarrow v_y$

Injection absorption



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Particle boundary conditions in Zeltron

Choice of boundary conditions (mod_input.f90)

```
! Specify the boundary conditions for the particles:
! 1. "PERIODIC": Periodic boundary conditions
! 2. "REFLECT": Particles are elastically reflected at the wall
! 3. "ABSORB": Particles are absorbed at the wall

CHARACTER(LEN=10), PARAMETER, PUBLIC :: BOUND_PART_XMIN="PERIODIC"
CHARACTER(LEN=10), PARAMETER, PUBLIC :: BOUND_PART_XMAX="PERIODIC"
CHARACTER(LEN=10), PARAMETER, PUBLIC :: BOUND_PART_YMIN="PERIODIC"
CHARACTER(LEN=10), PARAMETER, PUBLIC :: BOUND_PART_YMAX="PERIODIC"
```

Chunk from **SUBROUTINE** BOUNDARIES_PARTICLES *(mod_particles.f90)*

```
!***********************************************************************
! Case 1: x>xmax
!***********************************************************************
IF (x.GT.xmax) THEN

   ! Elastic reflection
   IF (BOUND_PART_XMAX.EQ."REFLECT") THEN
   x=2.0*xmax-x
   ux=-ux
   END IF

   ! Absorption
   IF (BOUND_PART_XMAX.EQ."ABSORB") THEN
   wt=0d0
   END IF

END IF
```


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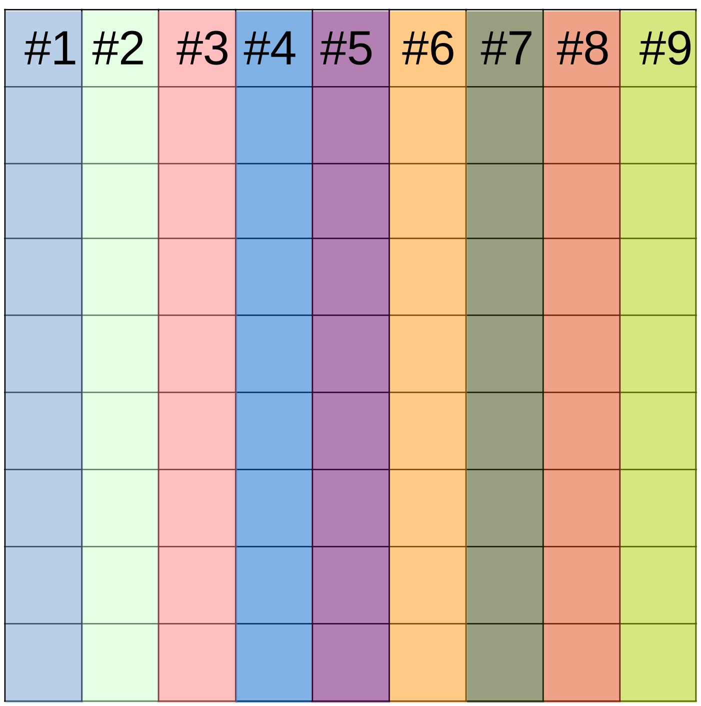
Parallelization: Domain decomposition

PIC code are really demanding in computing resources => **Need to parallelize the code!**

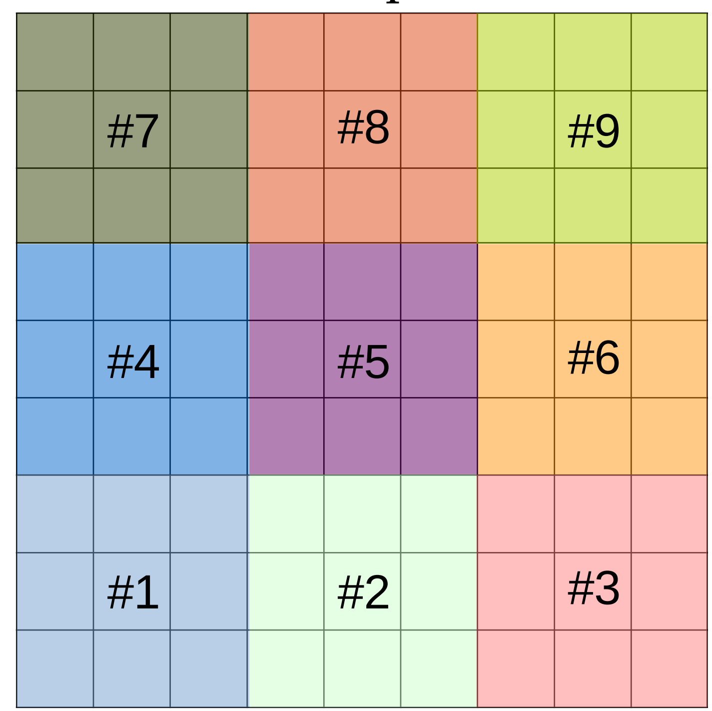
A common practice is to use the **Message Passing Interface (MPI)** library and the **domain decomposition technique.**

Example: Consider a 2D mesh 9x9 cells and 9 CPUs.

1D decomposition



2D decomposition



Applicable to an arbitrary number of CPUs

Choice decomposition depends on the problem

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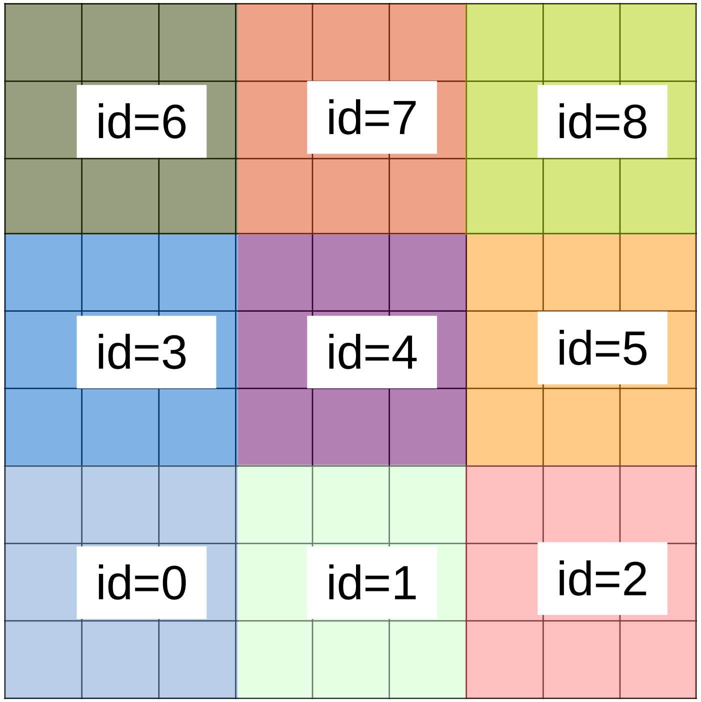
Define a topology

SUBROUTINE COM_TOPOLOGY in *mod_initial.f90*

```
! Initialization of the cartesian topology
periods(1)=.TRUE.
periods(2)=.TRUE.
reorder=.FALSE.
dims(1)=NPX ! Number of processors along X
dims(2)=NPY ! Number of processors along Y

! Creation of the dimension in each direction
CALL MPI_DIMS_CREATE(NPROC,2,dims,ierr)

! Creation of the topology
CALL MPI_CART_CREATE(MPI_COMM_WORLD,2,dims
,periods,reorder,COMM,ierr)

! To obtain the ID number of each process
CALL MPI_COMM_RANK(COMM,id,ierr)

! To obtain the coordinates of the process
CALL MPI_CART_COORDS(COMM,id,2,coords,ierr)
```

2D decomposition



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Local grids and arrays

Each processor has its own **local grid** and **local particle arrays** (*main.f90*)

```
! Spatial boundaries in the X-direction of each domain
DOUBLE PRECISION :: xminp,xmaxp

! Spatial boundaries in the Y-direction of each domain
DOUBLE PRECISION :: yminp,ymaxp

! Global nodal grid
DOUBLE PRECISION, DIMENSION(1:NX) :: xg
DOUBLE PRECISION, DIMENSION(1:NY) :: yg
! Nodal grid in each domain
DOUBLE PRECISION, DIMENSION(1:NXP) :: xgp
DOUBLE PRECISION, DIMENSION(1:NYP) :: ygp

! Yee grid in each domain
DOUBLE PRECISION, DIMENSION(1:NXP) :: xyeep
DOUBLE PRECISION, DIMENSION(1:NYP) :: yyeep
```

```
!==========================================================
! SPATIAL BOUNDARIES FOR EACH SUB-DOMAIN
!==========================================================

xminp=xmin+coords(1)*NCXP*dx
xmaxp=xminp+NCXP*dx

yminp=ymin+coords(2)*NCYP*dy
ymaxp=yminp+NCYP*dy
```

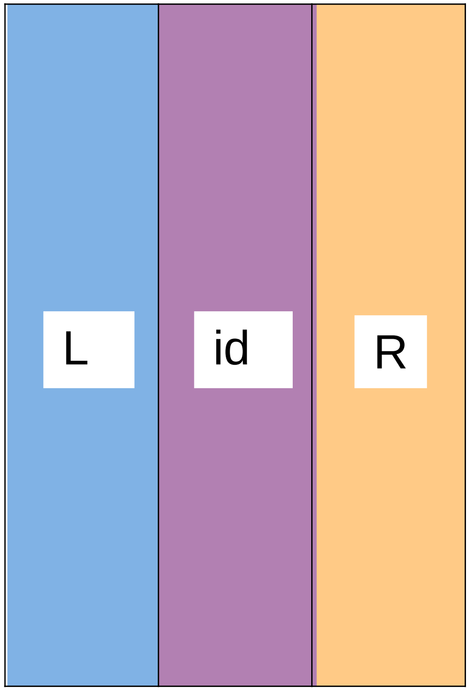
Neighbours

Once the topology defined, it is crutial that each processor knows its neighbours

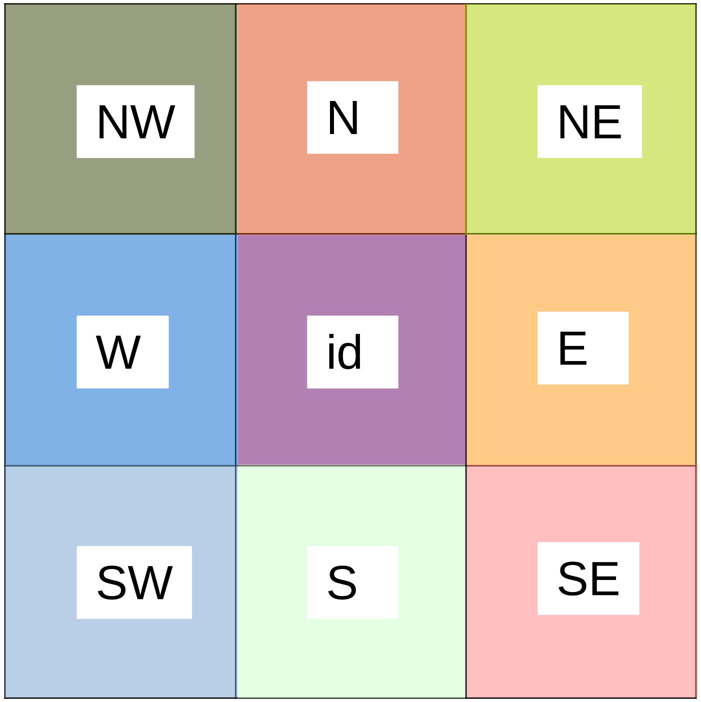
In Zeltron this information is contained in :

```
! ngh: neighbor array (1D)
INTEGER, DIMENSION(2) :: ngh

! ngh: neighbor array (2D)
INTEGER, DIMENSION(8) :: ngh

! ngh: neighbor array (3D)
INTEGER, DIMENSION(26) :: ngh
```

1D decomposition



2D decomposition



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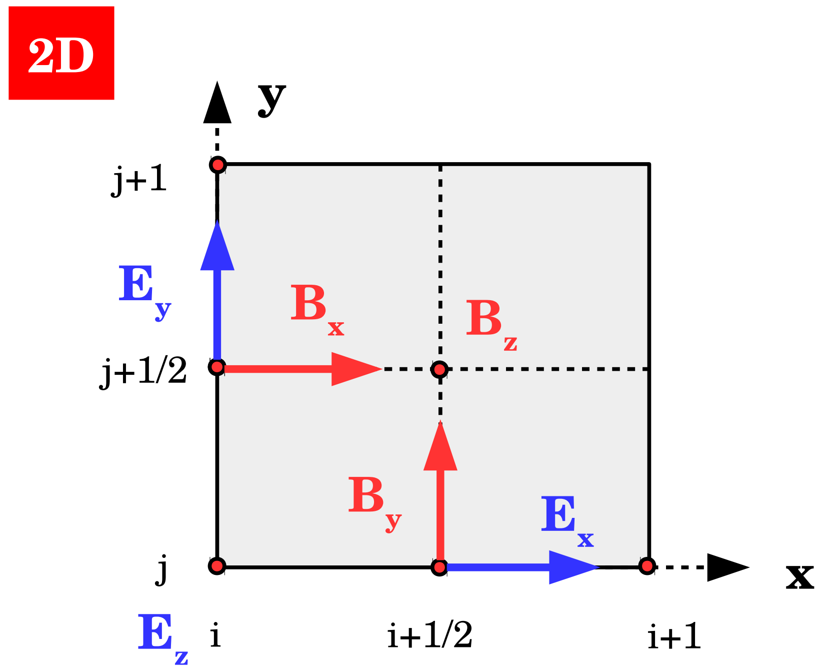
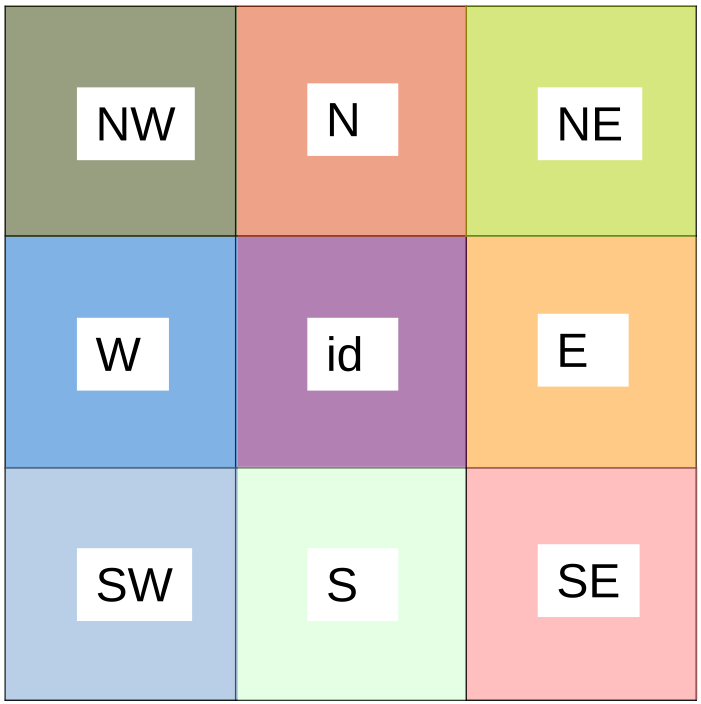
Communications between CPUs : Fields



2D decomposition



Example : We want to compute E field on the grid (**SUBROUTINE** FIELDS_NODES in *mod_fields.f90*)

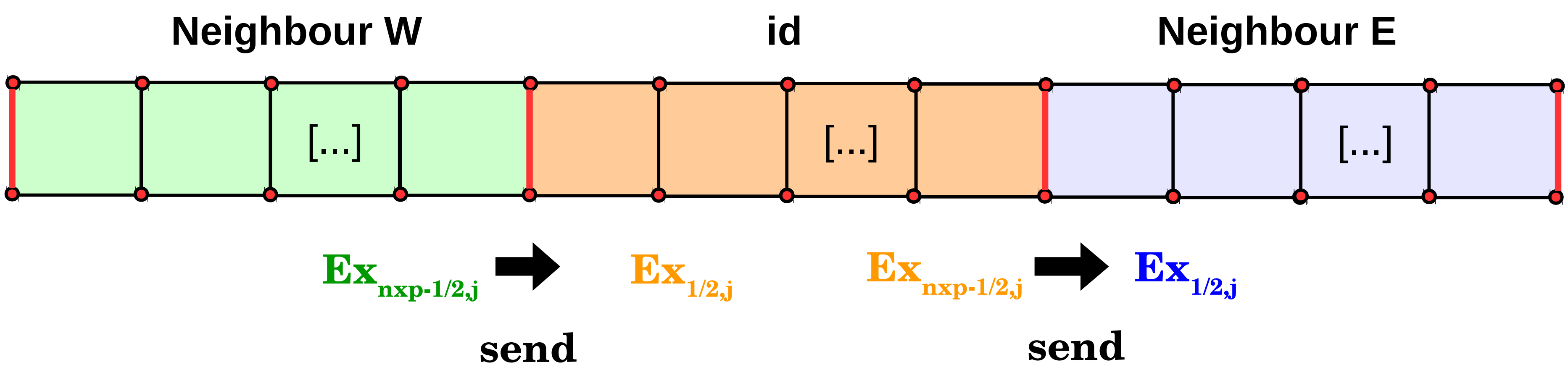
$$Exg_{i,j} = \frac{Ex_{i+1/2,j} + Ex_{i-1/2,j}}{2}$$

But we need $Ex_{-1/2,j}$ to compute $Ex_{0,j}$

This value is known by the neighbour W

=> W must send its values of $Ex_{nxp-1,j}$

Communications between CPUs : Fields



A very typical MPI "point-to-point" communication of a 1D array in Zeltron (from *mod_fields.f90*)

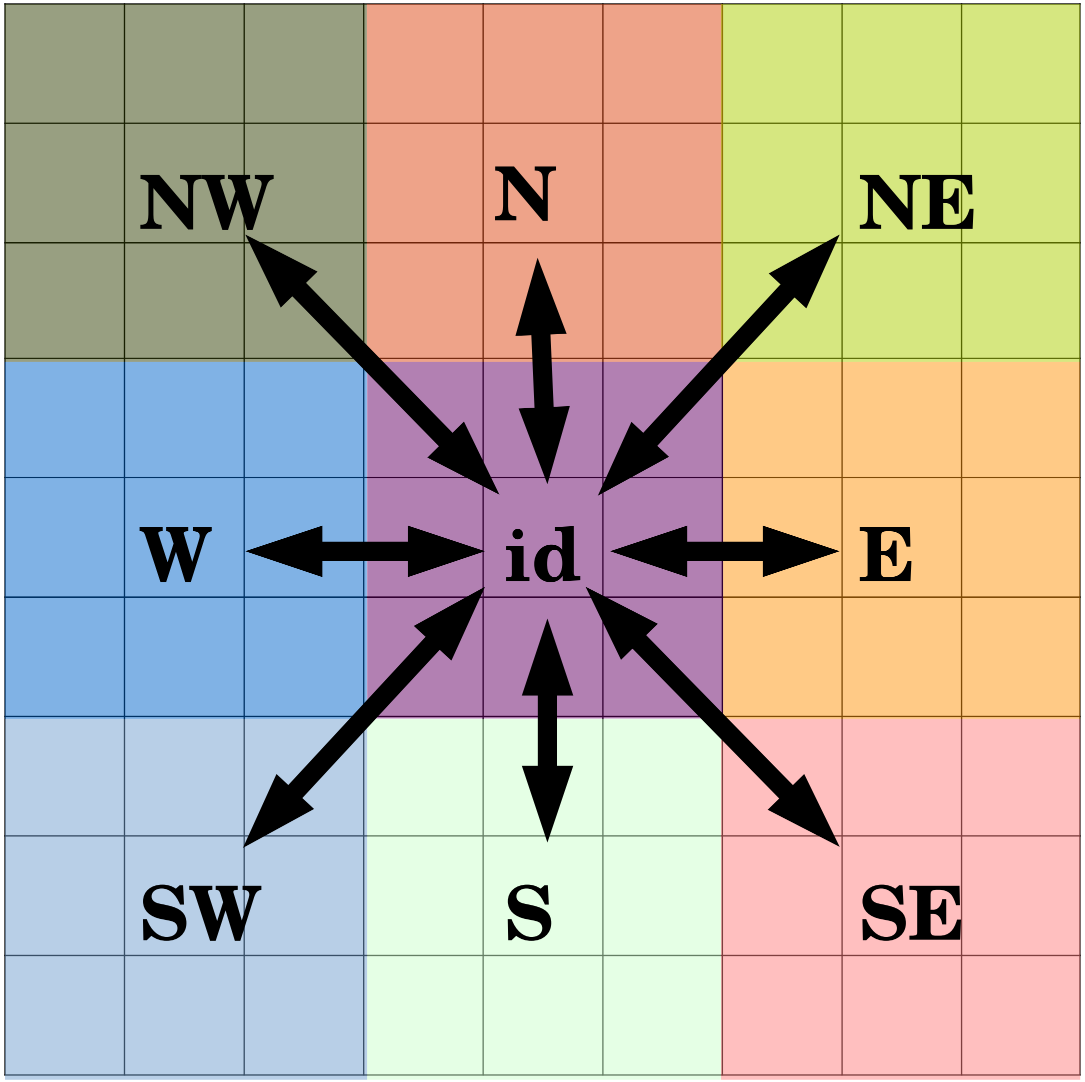
```
ALLOCATE(bufS2(1:NYP),bufR2(1:NYP))

bufS2=Ex(NXP-1,:)

IF (MOD(id,2).EQ.0) THEN
! For even CPU id
CALL MPI_SENDRECV(bufS2,NYP,MPI_DOUBLE_PRECISION,ngh(2),tag2,&
                  bufR2,NYP,MPI_DOUBLE_PRECISION,ngh(4),tag2,COMM,stat,ierr)
ELSE
! For odd CPU id
CALL MPI_SENDRECV(bufS2,NYP,MPI_DOUBLE_PRECISION,ngh(2),tag2,&
                  bufR2,NYP,MPI_DOUBLE_PRECISION,ngh(4),tag2,COMM,stat,ierr)
ENDIF
```

Communications between CPUs : Particles

MPI Communications

1D: Up to **2 / CPU** **2D:** Up to **8 / CPU** **3D:** Up to **26 / CPU**

Example: 2D decomposition



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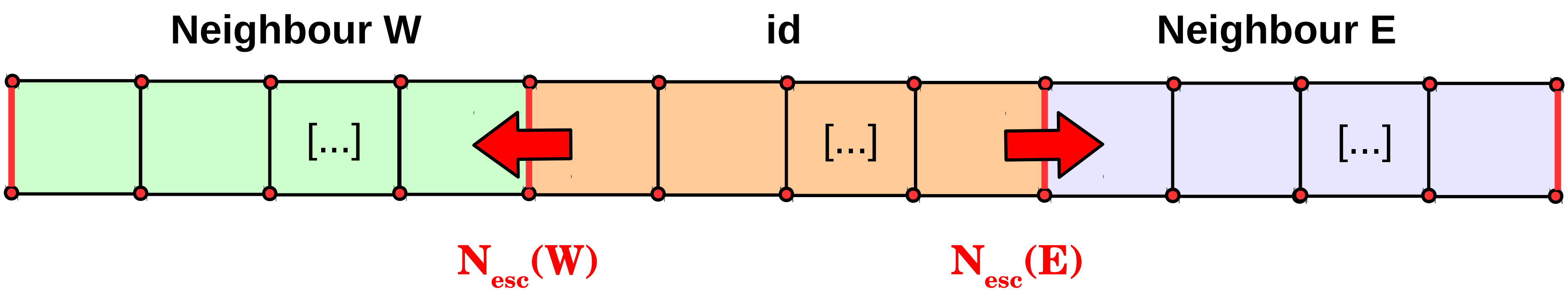
Communications between CPUs : Particles

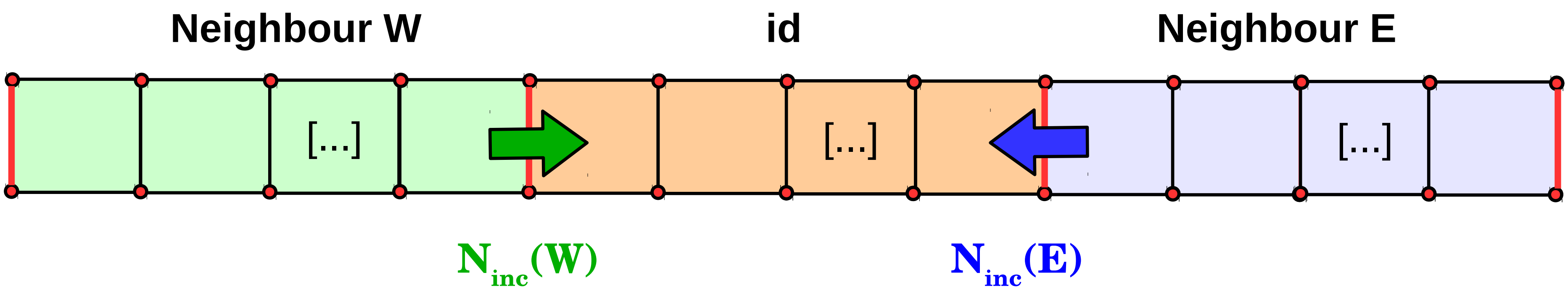
Steps for exchanging particles

SUBROUTINE COM_PARTICLES (*mod_motion.f90*)

Step 1 : Count all particles leaving the processor domain towards the neighbouring processors.



Step 2 : Ask the neighbours how many particles are leaving their domains towards processor id.



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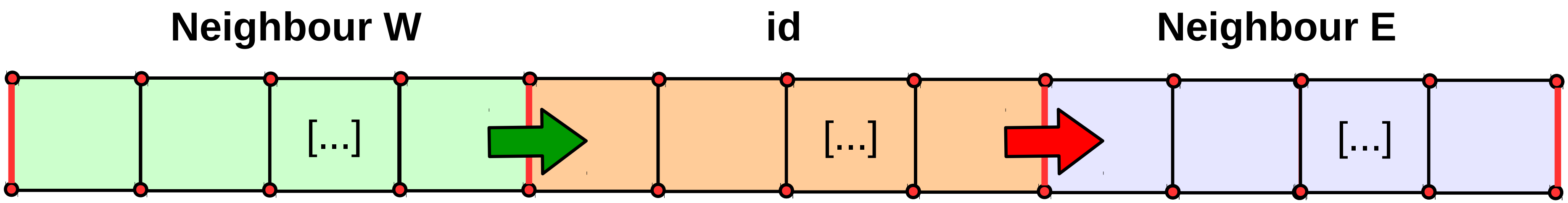
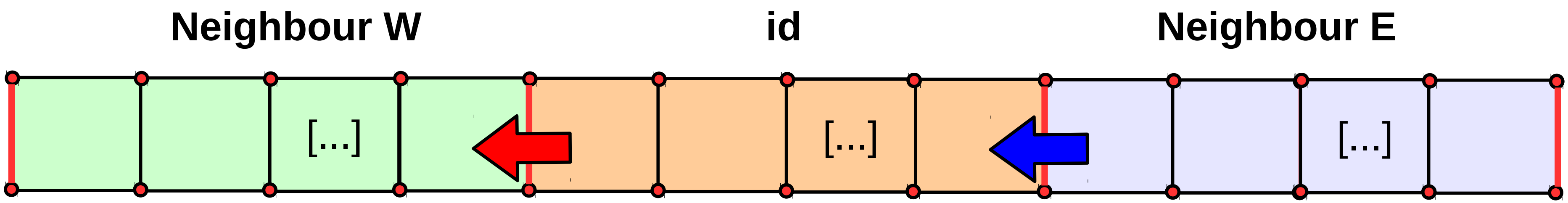
Communications between CPUs : Particles

Step 3: Exchange particle data (x,y,z,ux,uy,uz,wgt,tag,...)



bufRW => pcl[N_{inc}(W)] **bufSE => pcl[N_{esc}(E)]**

```
CALL MPI_SENDRECV(bufSE,NESC(2)*11,MPI_DOUBLE_PRECISION,ngh(2),tag2,&
     bufRW,NINC(4)*11,MPI_DOUBLE_PRECISION,ngh(4),tag2,COMM,stat,ierr)
```



bufSW => pcl[N_{esc}(W)] **bufSE => pcl[N_{inc}(E)]**

```
CALL MPI_SENDRECV(bufSW,NESC(4)*11,MPI_DOUBLE_PRECISION,ngh(4),tag4,&
     bufRE,NINC(2)*11,MPI_DOUBLE_PRECISION,ngh(2),tag4,COMM,stat,ierr)
```

Step 4: Resize particle array to update the content of particles in each domain.

$$pcl\left(N_{new}\right) \leftarrow pcl\left(N_{old} - N_{esc} + N_{inc}\right)$$

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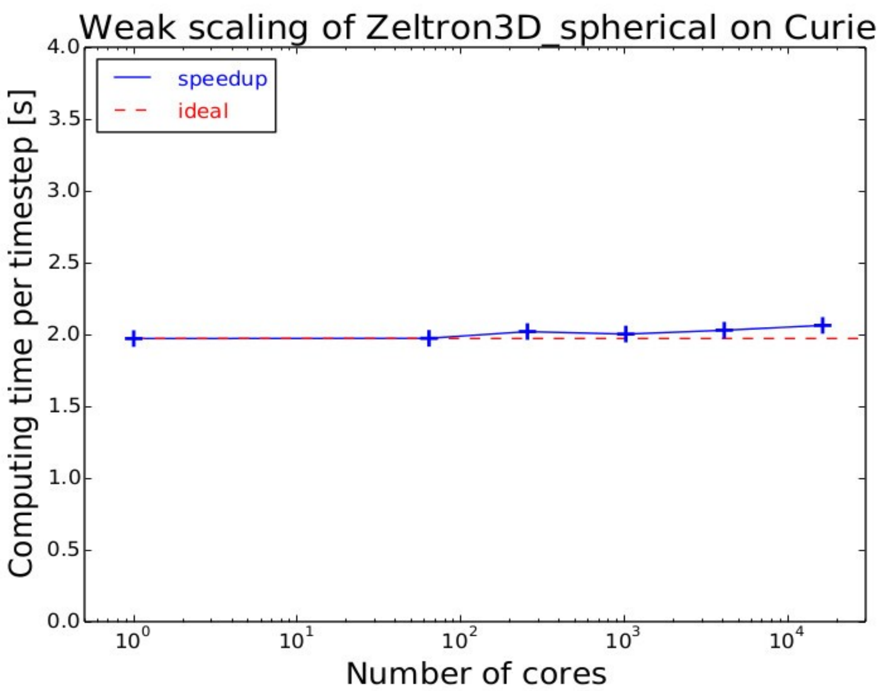
PIC codes scale well to large number of CPUs

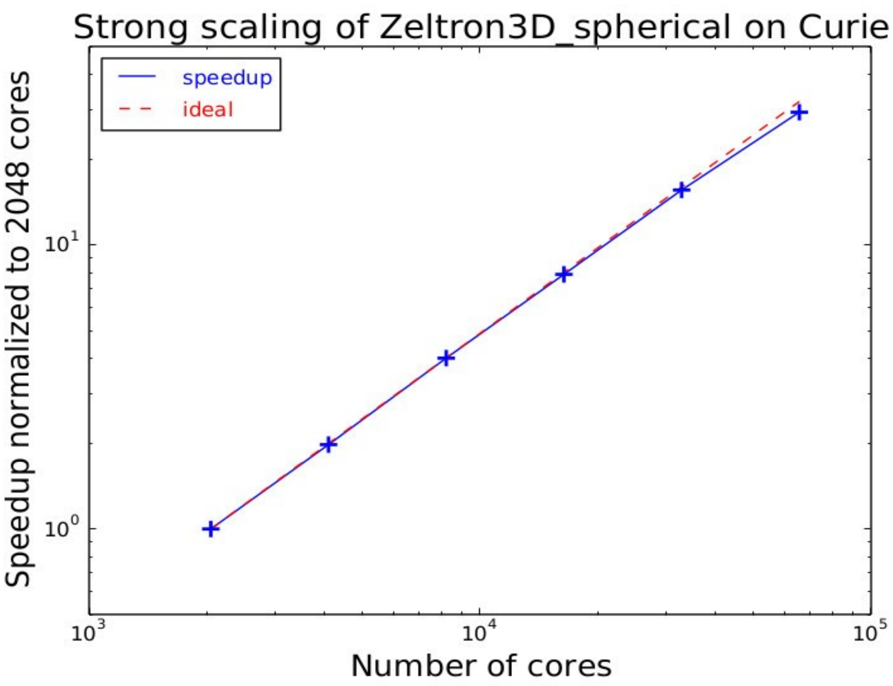
The era of **High-Performance Computing!** Today ~> **10^6 CPUs**

See http://www.top500.org/

Weak scaling



Strong scaling



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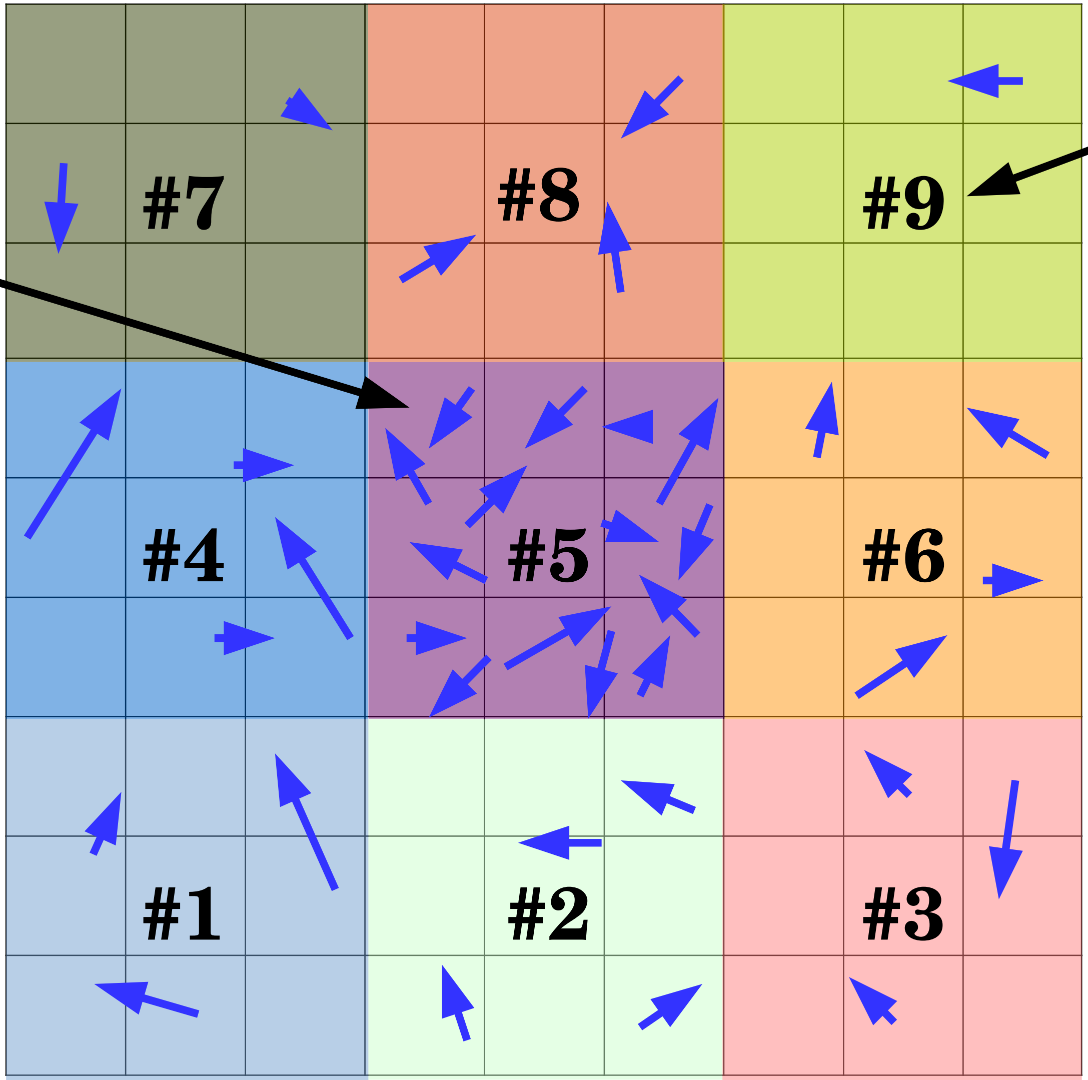
Load balancing issues

Computing time (without communications): ~ 90% **particles**, ~10% **fields**

Many particles
Processor #5 is
slowing down all
the others



Few particles
Processor #9 is
waiting for all the
others

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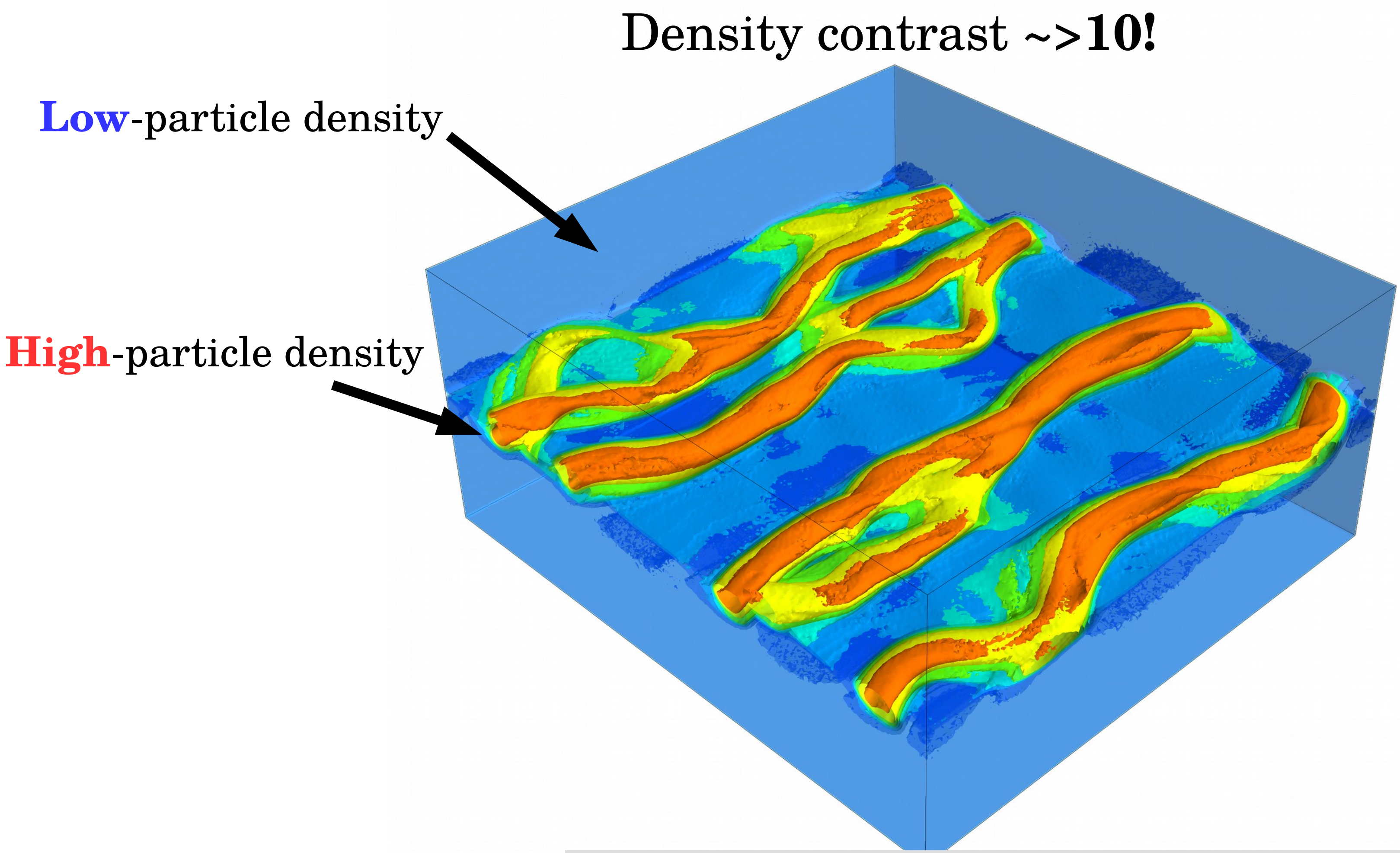
A specific example: a reconnecting layer



Some solutions:

- Appropriate domain decomposition
- Dynamical changes of the decomposition
- Varying particle weights
- Hybrid code: MPI-OpenMP

…

Another specific example: a shock

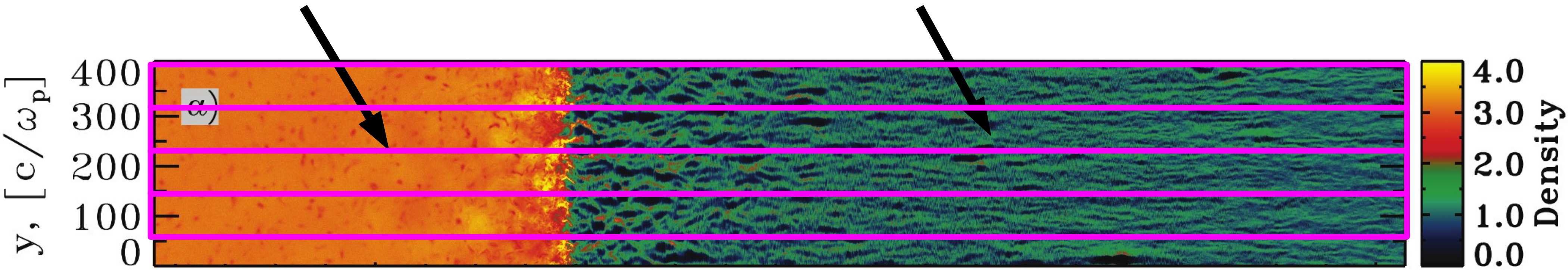
Density contrast ~**4**

High-particle density

Downstream, shocked flow

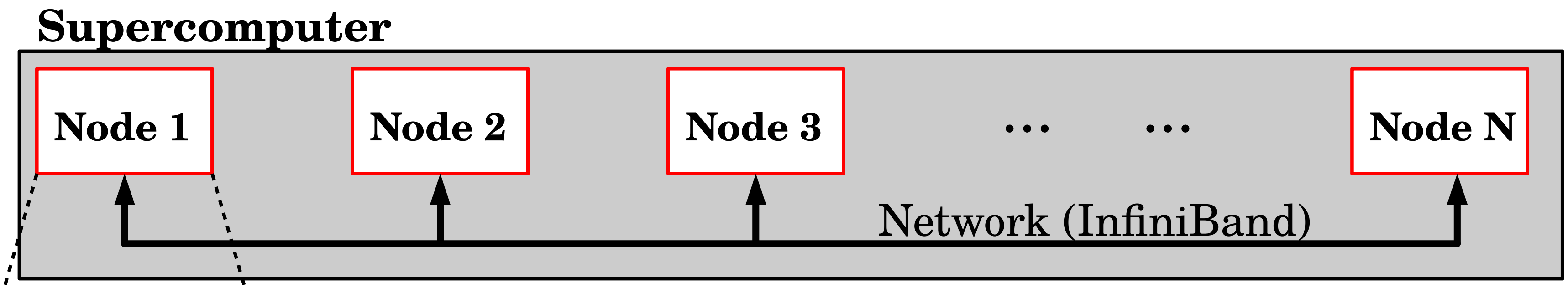
Low-particle density

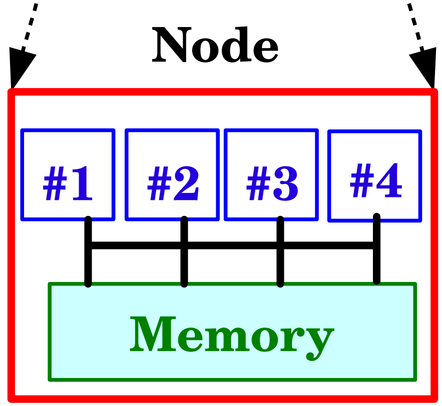
Upstream, unshocked plasma



1D decomposition is appropriate here, but maximum number of cores is **limited.**

Hybrid parallelization: MPI-OpenMP

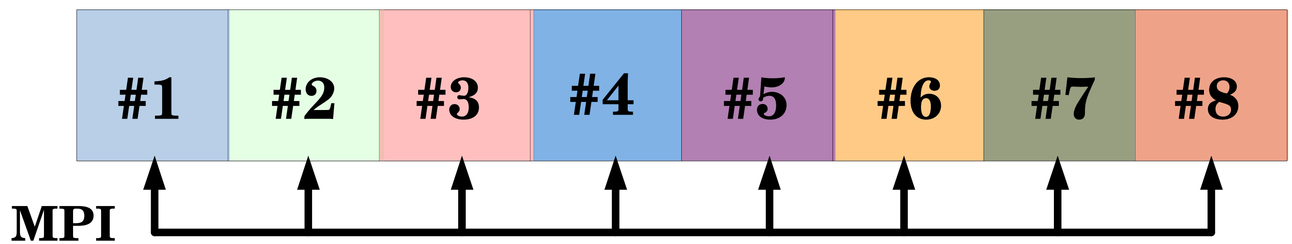




Memory is shared
within a node

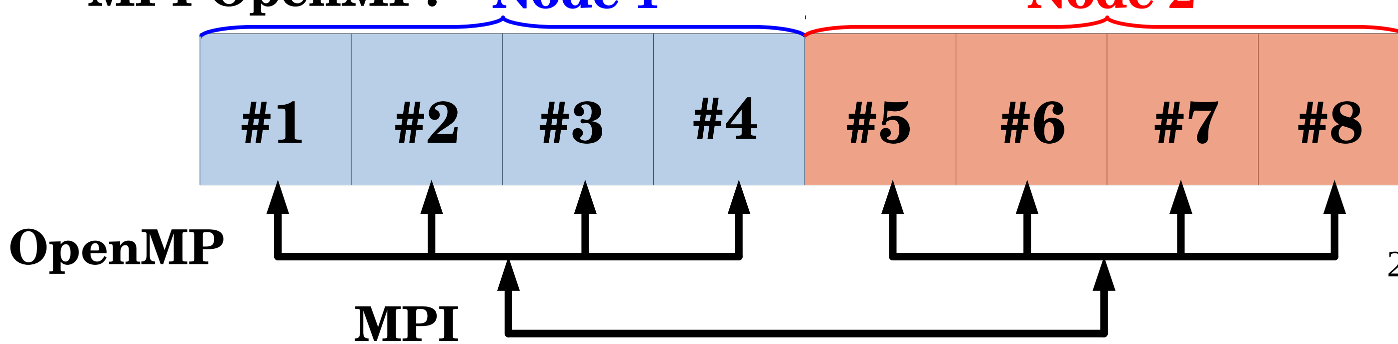
Example: 2 nodes, 4 processors per node. 1D decomposition

- **Pure MPI:**



The particle loop can be parallelized with OpenMP within a node.
=> Bigger domain, better load balancing.

- **MPI-OpenMP:**



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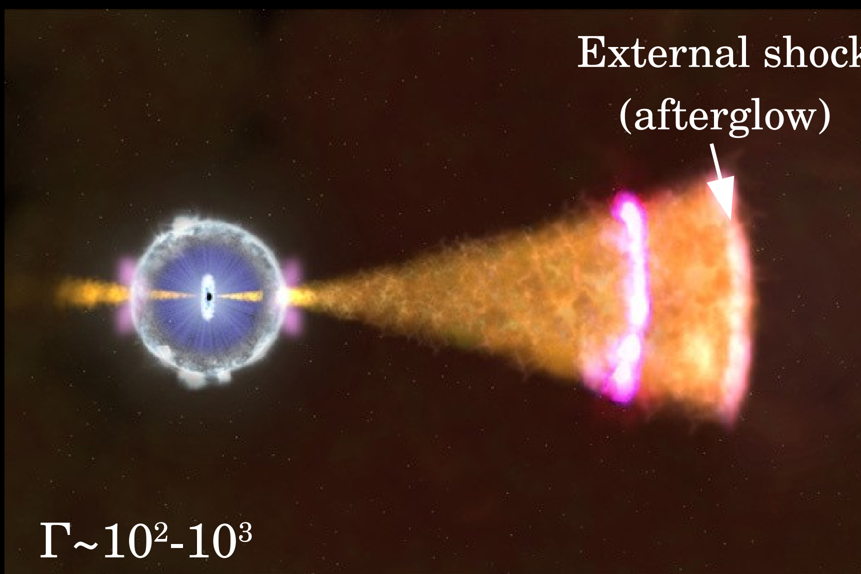
Hands-on III: Relativistic collisionless shocks

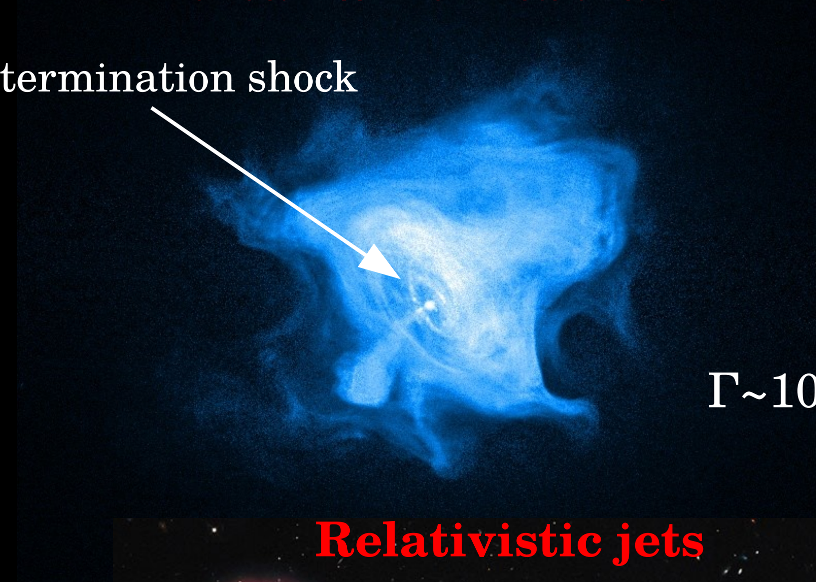
Collisionless shock sounds counter-intuitive. To form a shock we need collisions, something that thermalizes the flow (randomize particle's velocity). In collisionless shocks, waves and magnetic irregularities effectively collide with particles.

Main astrophysical applications:

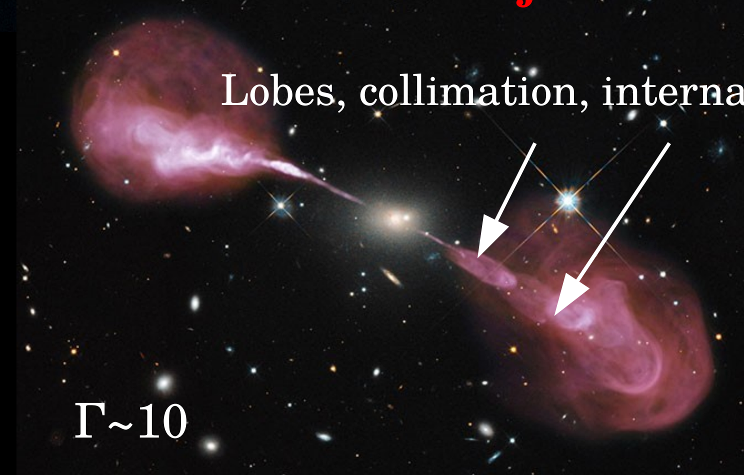
Gamma-ray bursts



Pulsar Wind Nebulae



Relativistic jets



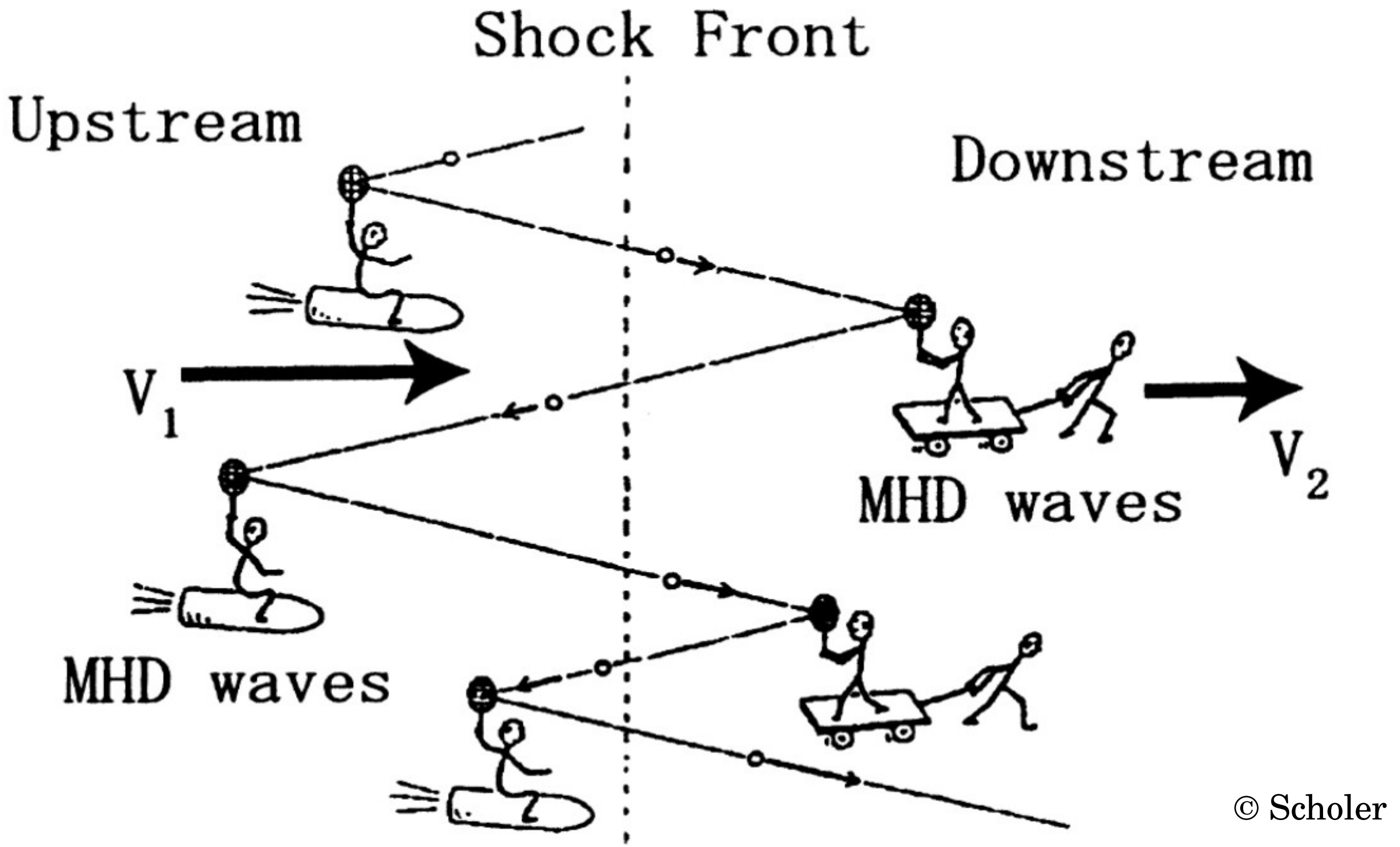
How efficient at accelerating particles?

What are the main acceleration mechanisms?

Diffusive shock acceleration

Axford 1977, Krymsky 1977, Blandford & Ostriker 1978, Bell 1978

See e.g. Pelletier et al. 2017 for a review



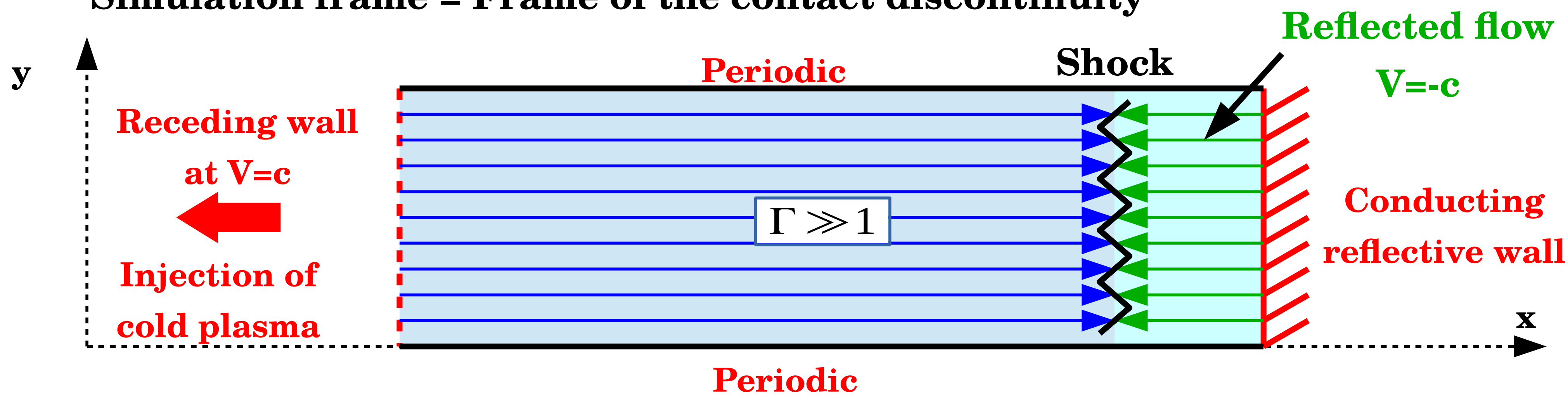
Prediction: generates broad steep (~-2) power-laws, but needs strong plasma turbulence at kinetic scales on both downstream and upstream!

Does it work?

Recent studies are based on ab-initio particle-in-cell (PIC) simulations

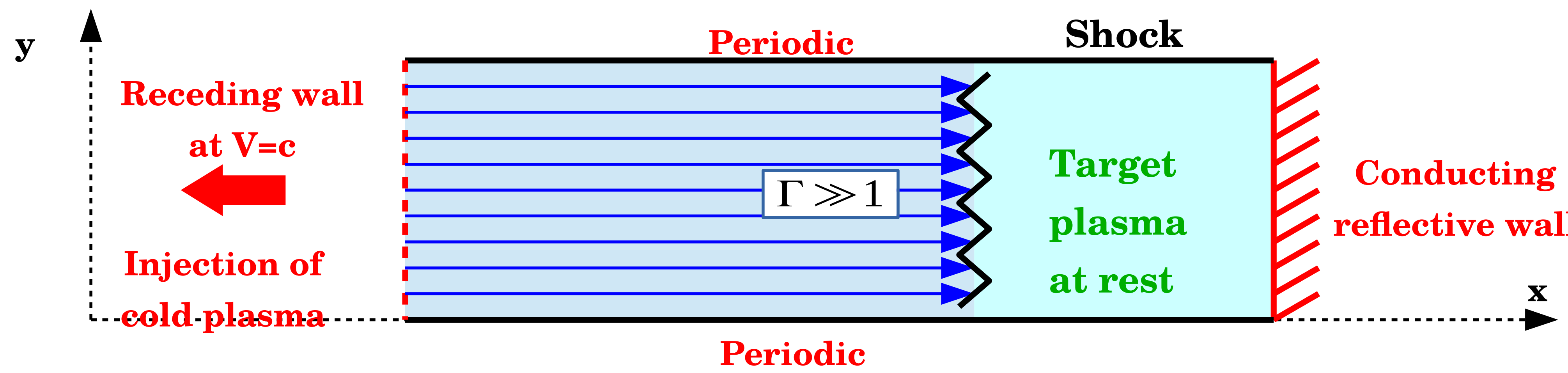
The usual numerical setups

Simulation frame = Frame of the contact discontinuity



Good setup to follow the formation of one shock only (the reverse shock)

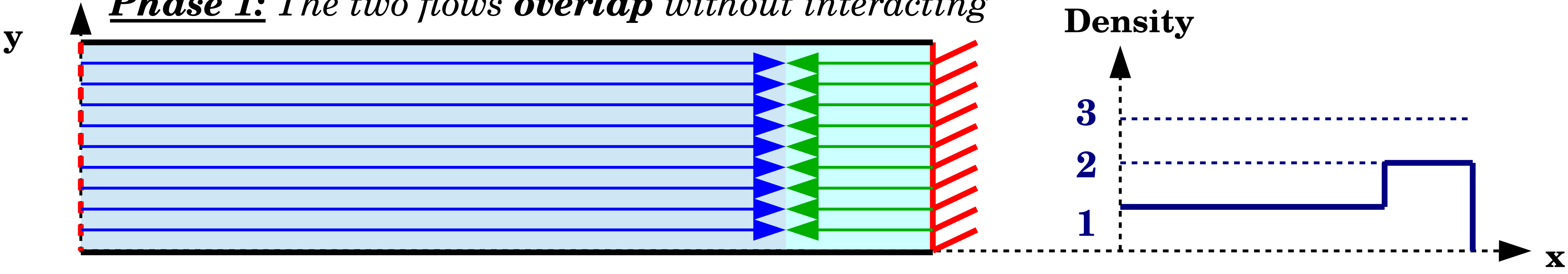
Simulation frame = Frame of the downstream flow



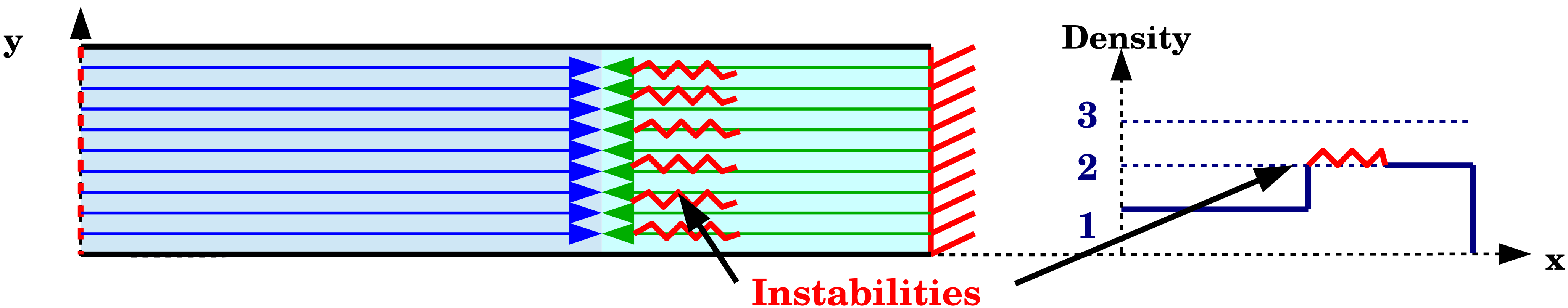
Good setup to follow the formation of all the shocks plus contact discontinuity

Unmagnetized collisionless shock formation

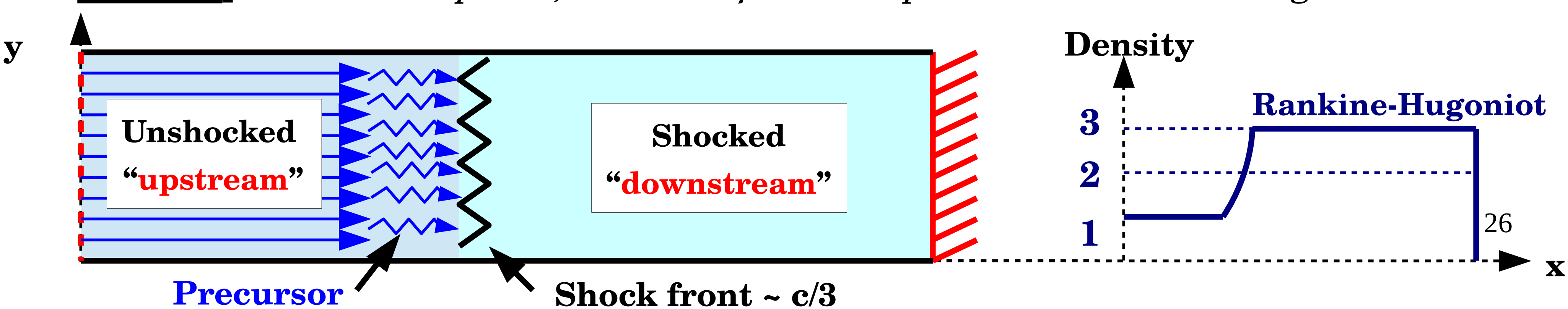
Phase 1: *The two flows* ***overlap*** *without interacting*



Phase 2: *Electromagnetic counter-streaming* ***instabilities*** *grows (linear phase)*



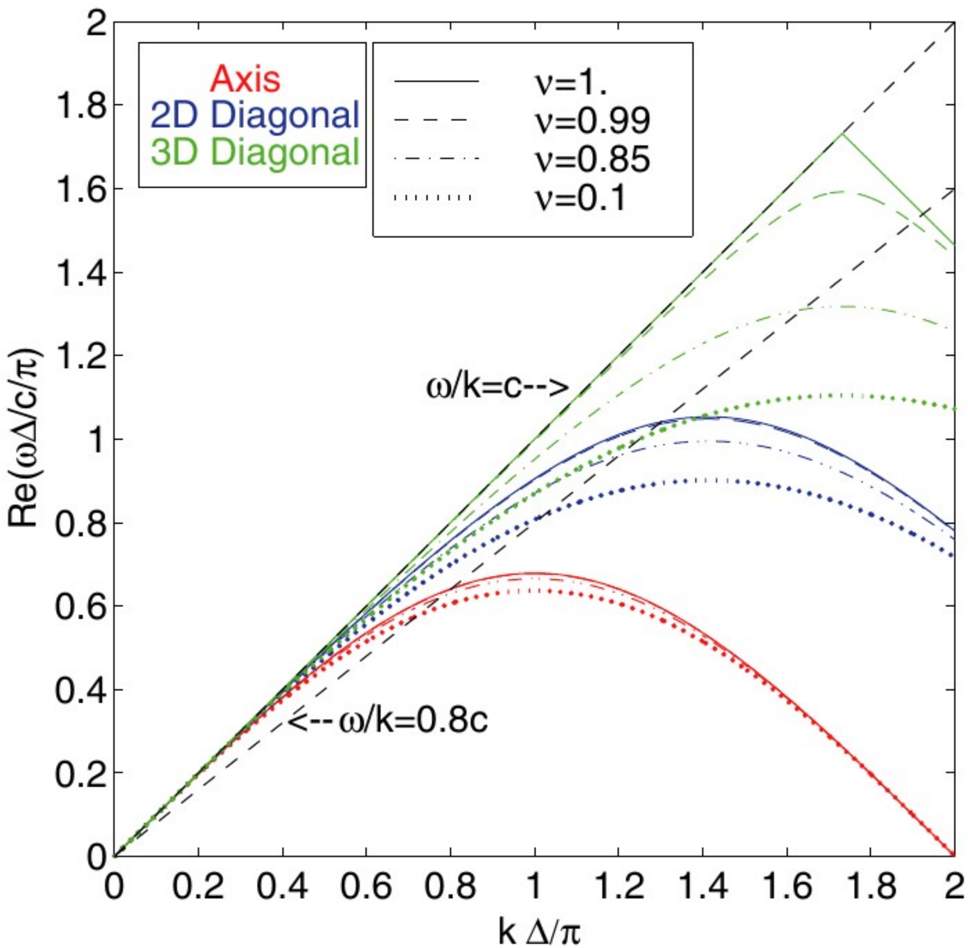
Phase 3: ***Non-linear*** *phase, the shock form and particle acceleration begins*



Numerical Cherenkov radiation

Numerical dispersion relation (Lecture I)

$$\left[\frac{1}{c\Delta t}\sin\left(\frac{\omega\Delta t}{2}\right)\right]^2=\left[\frac{1}{\Delta x}\sin\left(\frac{k_x\Delta x}{2}\right)\right]^2+\left[\frac{1}{\Delta y}\sin\left(\frac{k_y\Delta y}{2}\right)\right]^2$$



A.D. Greenwood et al. / Journal of Computational Physics 201 (2004) 665–684

Instead of:

$$\frac{\omega^2}{c^2}=k_x^2+k_y^2$$

If relativistic cold plasma beam v~c

=> Numerical Chenrenkov radiation

Plasma beam heats up !

$\Gamma\approx 1$ => Non-relatvistic shock

How to mitigate :

- Filtering
- Higher order schemes for derivatives

See e.g. *Greenwood + 2004*