ISSS-15 + IPELS-16

RUB

SEMI-IMPLICIT PARTICLE IN CELL METHODS

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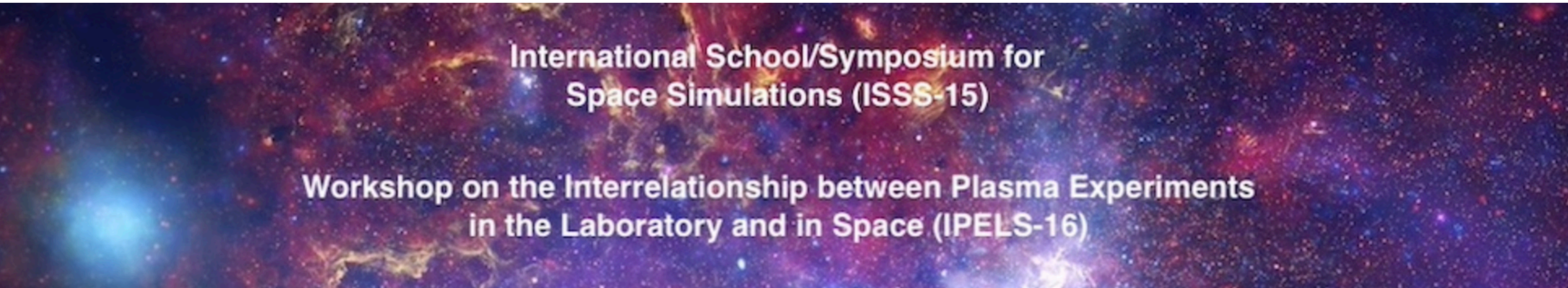

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COMPUTATIONAL PLASMA PHYSICS @ RUB

M.E. Innocenti: mariaelena.innocenti@rub.de

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- ✦Semi-implicit Particle-In-Cell, HPC
- ✦Advanced PIC methods: MLMD, Expanding Box semi-implicit PIC

J. Dreher: juergen.dreher@ruhr-uni-bochum.de

- ✦(Hall-)MHD and fluid modeling
- ✦Magnetic reconnection in space plasmas
- ✦Mesh-adaptive computation, HPC code development

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- ✦Robust structure-preserving PIC, explicit and implicit
- ✦HPC
- ✦Kinetic processes in fusion

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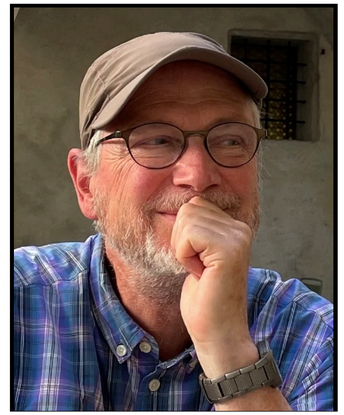
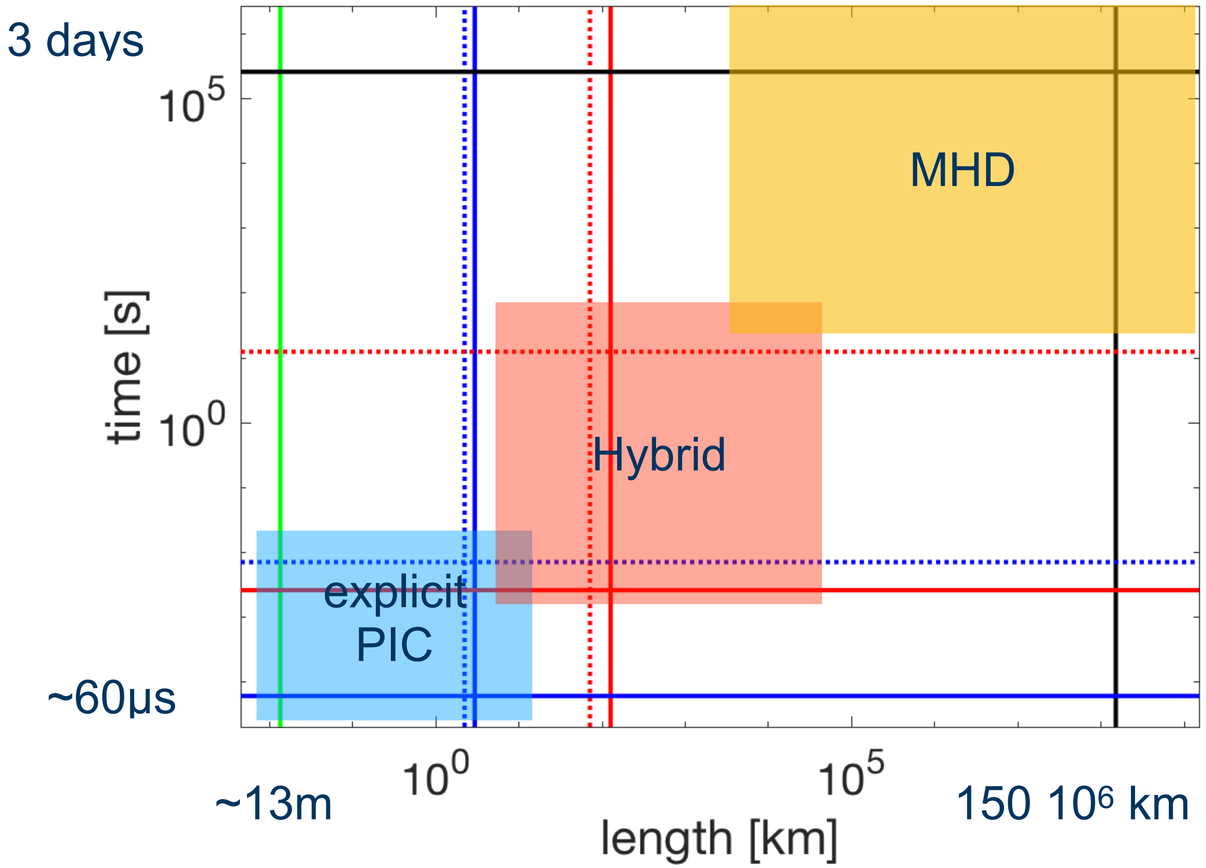
- ✦Reconnection and turbulence
- ✦Multiphysics simulations
- ✦Coupling adaptively 2 fluid 5/ 10 moment codes with Vlasov



2. SPACE SIMULATIONS: SCALES & CHALLENGES

NUMERICAL METHODS & SCALE SEPARATIONS IN SPACE PHYSICS



INTERPLANETARY SPACE

λ_D	Debye length
r_e	electron gyroradius (:)
d_e	electron skin depth
r_i	ion gyroradius (:)
d_i	ion skin depth
L	1 AU
ω_{pe}^{-1}	electron plasma f $^{-1}$
ω_{pI}^{-1}	ion plasma f $^{-1}$
Ω_e^{-1}	electron gyro f^{-1} (:)
Ω_I^{-1}	ion gyro f^{-1} (:)
T	3 days

ASSOCIATE NUMERICAL METHODS TO BOXES

MagnetoHydroDynamics (MHD):

✓ ions & electrons are simulated as fluid: kinetic processes must be negligible

✓ best suited for: global-scale processes

✓ low computational cost per unit volume (kinetic scales not resolved)

Hybrid:

✓ ions are simulated as particles, electrons are a massless fluid: plasma must be quasi-neutral, electron-scale kinetic processes must be negligible

✓ best suited for: ion scale processes

✓ moderate computational cost per unit volume (need to resolve smallest, fastest *ion* scales)

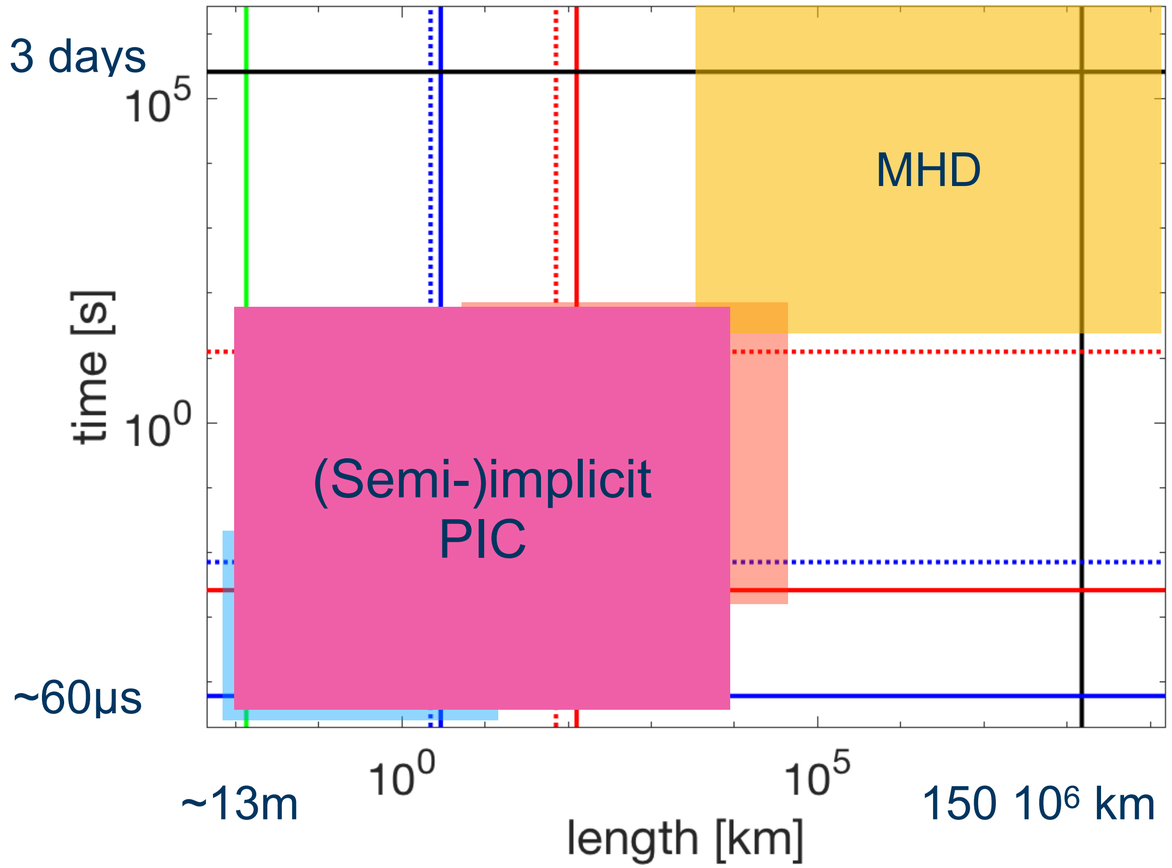
Explicit Particle in Cell, PIC:

✓ electrons and ions are simulated as particles: no assumptions on the state of the plasma

✓ best suited for: electron scale processes

✓ high computational cost per volume (need to resolve smallest, fastest *electron* scales)

WHY SEMI-IMPLICIT PIC?



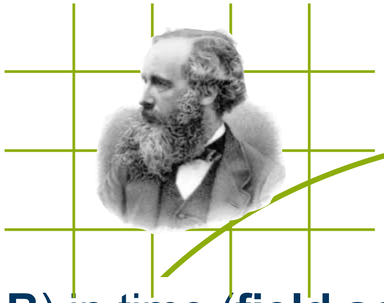
(Semi-)Implicit PIC:

- ✓electrons and ions are treated as particles: no assumptions on the state of the plasma
- ✓can address either electron or ion scale processes, *depending on resolution of choice*
- ✓lower computational cost than explicit PIC, *if resolution is appropriately chosen* (can step over the smallest, fastest electron scales)
- ✓a word of caution: processes which are not resolved are captured *qualitatively*, not *quantitatively*

3. PIC METHODS: A SUMMARY

FIELDS & PARTICLES IN PIC METHODS

Two main “systems”: **fields** and **particles**



q_i, m_i: particle charge and mass

To advance **fields** (**E** & **B**) in time (**field solver**):

Some combination of **Maxwell’s equation**

Gauss $\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}$ → density

Faraday $\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$

Gauss for magn $\nabla \cdot \mathbf{B} = 0$

Ampere $\nabla \times \mathbf{B} = \mu_0 \mathbf{J} + \mu_0 \epsilon_0 \frac{\partial \mathbf{E}}{\partial t}$

current

Fields live on a **grid**

To advance **particle** i in time (**particle mover**):

Newton’s equations

$$\frac{d\mathbf{x}_i}{dt} = \mathbf{v}_i$$

$$\frac{d\mathbf{v}_i}{dt} = \frac{q_i}{m_i}(\mathbf{E}_i + \mathbf{v}_i \times \mathbf{B}_i)$$

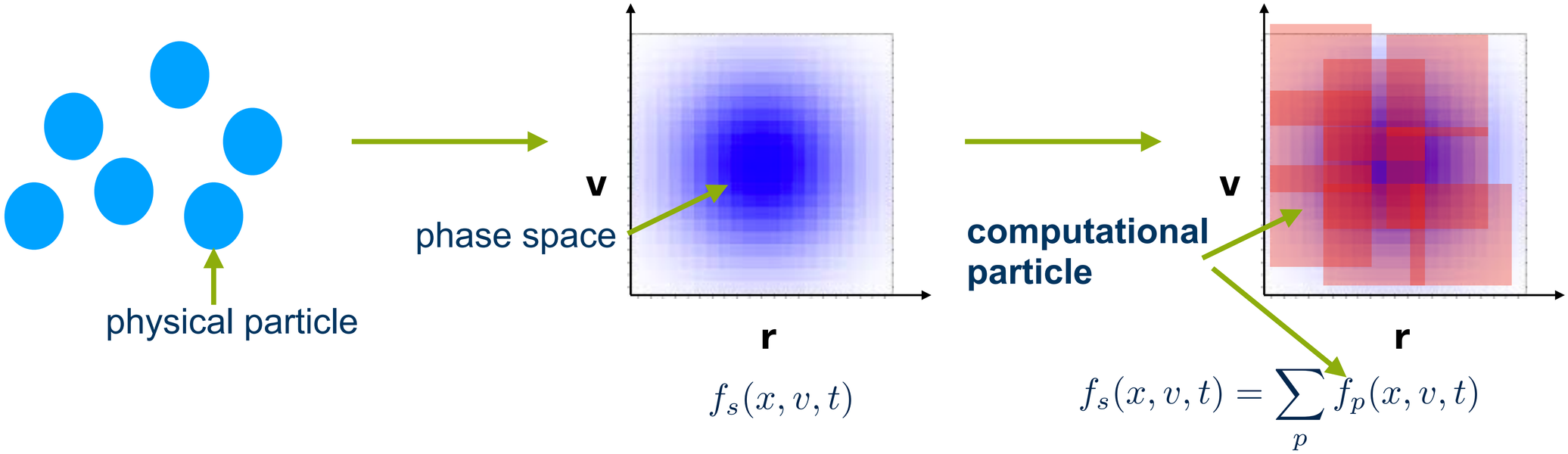
fields *at the particle position*

Particles move in the **continuum;** they accumulate density and current to the grid; they require fields at particle position

Focus on **particles**

FROM PHYSICAL PARTICLES TO COMPUTATIONAL PARTICLES

How to reduce the computational cost of simulating real, physical particles?



"shape" of the computational particle:

$$f_p(x,v,t) = N_p S_x(x - x_p(t)) S_v(v - v_p(t))$$

# of real particles in the CP — **Shape functions** in x & v

In PIC we work with **computational, super-particles**, not with real particles

SHAPE FUNCTIONS OF COMPUTATIONAL PARTICLES & THE GRID

Usual choices:

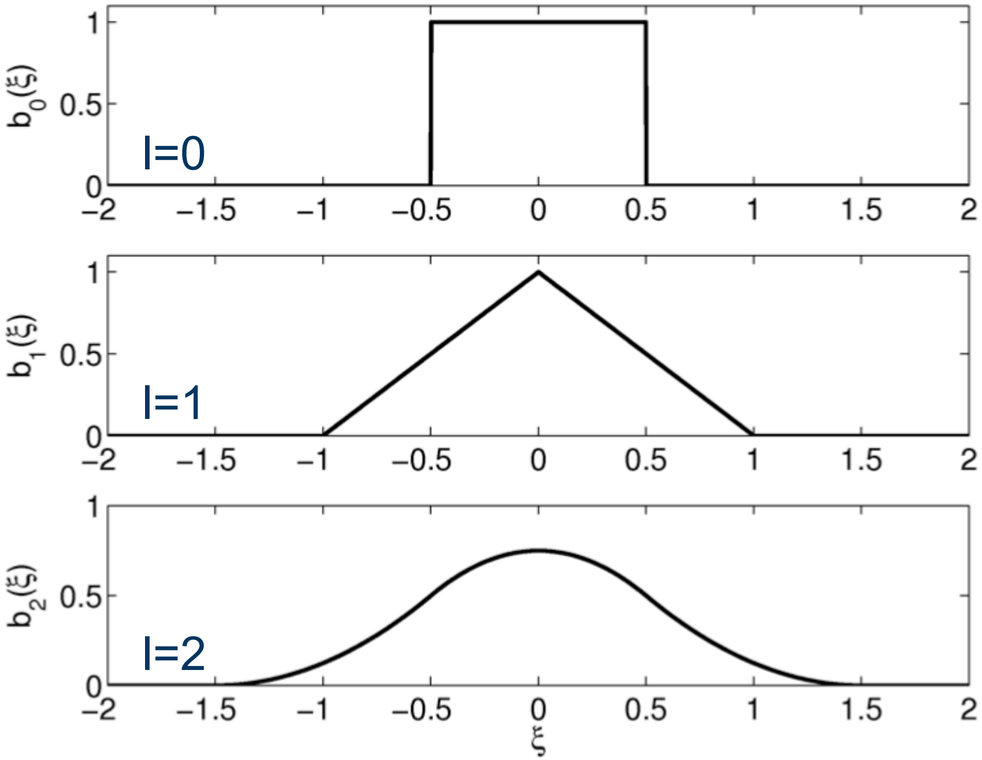
1. For v: delta function: $S_v\left(v - v_p\right) = \delta\left(v - v_p\right)$

2. For x: b-splines: $S_x(x - x_p) = b_l\left(\dfrac{x - x_p}{\Delta p}\right)$

support of the particle

$$b_0(\xi) = \begin{cases} 1 & \text{if } |\xi| < 1/2 \\ 0 & \text{otherwise} \end{cases} \qquad b_l(\xi) = \int_{-\infty}^{\infty} d\xi' b_0(\xi - \xi') b_{l-1}(\xi')$$

Higher order splines: higher computational cost, smoother solution



Particles with shape function S deposit moments to the grid through interpolation function W, the b-spline of one order higher

Example: density

Important for later!

continuum: $\rho = \sum_s \rho_s = q_s \sum_p N_p S_x(x - x_p)$

@ grid points: $\rho_i = \sum_p \dfrac{q_p}{\Delta x} W(x_i - x_p)$

A CYCLE OF ANY PIC CODE

Fields

Computational particles

Field to particle, F2P, interpolation:

$$\mathbf{E}, \mathbf{B} \rightarrow \mathbf{E}_i, \mathbf{B}_i$$

$$E_p = \sum_i E_i W(x_i - x_p)$$

Calculated at grid points, Eulerian framework

Field solver:

$$\mathbf{E}_i^n, \mathbf{B}_i^n \rightarrow \mathbf{E}_i^{n+1}, \mathbf{B}_i^{n+1}$$

Particle mover:

$$\mathbf{x}_p^n, \mathbf{v}_p^n \rightarrow \mathbf{x}_p^{n+1}, \mathbf{v}_p^{n+1}$$

Moved in the continuum, Lagrangian framework

$$\rho_i = \sum_p \frac{q_p}{\Delta x} W(x_i - x_p)$$

Moment gathering, P2F:

$$\mathbf{x}_p, \mathbf{v}_p \rightarrow \rho_i, \mathbf{J}_i$$

We know how to do the F2P and P2F steps, let's look at temporal advancement for F and P

4. TEMPORAL DISCRETIZATION OF ODE'S

TEMPORAL DISCRETIZATION OF ORDINARY DIFFERENTIAL EQ., ODE

We want to solve the ODE: $$\frac{df(t)}{dt} = G\left(f(t), t\right)$$

Discretization of the independent variable (time): step Δt, $t_n = t_0 + n\Delta t$

Evaluation of the function at discrete times: $f_n := f(t_n) = f(t_0 + n\Delta t)$

To step from time n to time n+1: $$\int_{t_n}^{t_{n+1}} df(t) = \int_{t_n}^{t_{n+1}} G(f(t), t)dt \qquad f_{n+1} = f_n + \int_{t_n}^{t_{n+1}} G(f(t), t)dt$$

:=I

Now we have to choose which method to use to calculate I:

- **Explicit discretization,** forward Euler
- **Implicit discretization,** backward Euler
- **θ, trapezoidal, Crank-Nicholson**

EXPLICIT vs IMPLICIT DISCRETIZATION

✓**Explicit discretization:** $$I = \int_{t_n}^{t_{n+1}} G(f(t),t)dt = \Delta t G(f_n, t_n) + \mathcal{O}\left(\Delta t^2\right)$$

Local integration error

Error to integrate up to time T=nΔt (global error): $T/\Delta t \times \mathcal{O}\left(\Delta t^2\right) = \mathcal{O}\left(\Delta t\right)$

$$f_{n+1} = f_n + \Delta t G(f_n, t_n)$$

First order accurate,
system energy tends to **increase**

✓**Implicit discretization:** $$f_{n+1} = f_n + \Delta t G(f_{n+1}, t_{n+1})$$

First order accurate,
System energy tends to **decrease**

Then the eq has to be recast as: $$f_{n+1} = H(f_n, t_n)$$

Θ-, TRAPEZOIDAL AND CRANK-NICHOLSON METHODS

✓**θ-methods:** continuous transition between forward and backward Euler

$$f_{n+1} = f_n + \Delta t \left[(1-\theta) G(f_n, t_n) + \theta G(f_{n+1}, t_{n+1}) \right]$$

- θ=0 → forward Euler, O(Δt)
- θ=1 → backward Euler, O(Δt)
- θ=1/2 → **trapezoidal method**, O(Δt²)

With θ=1/2, **second order** accurate

Crank-Nicholson:

$$f_{n+1} = f_n + \Delta t G \left(\frac{f_n + f_{n+1}}{2}, \frac{t_n + t_{n+1}}{2} \right)$$

θ-schemes with θ=1/2 and C-N are the same for linear G's

EXAMPLE: HARMONIC OSCILLATOR

Harmonic oscillator, with coordinates p and q

$$q'(t) = \omega p(t)$$
$$p'(t) = -\omega q(t)$$

Stability analysis: system **eigenvalues**!

✓Explicit discretization

$$q_{n+1} = q_n + \omega \Delta t p_n$$
$$p_{n+1} = p_n - \omega \Delta t q_n$$

Stability analysis: always unstable

$$|\lambda_{1,2}| = \sqrt{\Re(\lambda_{1,2})^2 + \Im(\lambda_{1,2})^2} = \sqrt{1 + (\omega \Delta t)^2} > 1$$

✓Implicit discretization

$$q_{n+1} = q_n + \omega \Delta t p_{n+1}$$
$$p_{n+1} = p_n - \omega \Delta t q_{n+1}$$

$$\begin{bmatrix} q_{n+1} \\ p_{n+1} \end{bmatrix} = \frac{1}{1 + \omega^2 \Delta t^2} \begin{bmatrix} 1 & \omega \Delta t \\ -\omega \Delta t & 1 \end{bmatrix} \begin{bmatrix} q_n \\ p_n \end{bmatrix}$$

Stability analysis: always stable

$$|\lambda_{1,2}| < 1$$

✓Trapezoidal discretization, θ=1/2

$$q_{n+1} = q_n + \frac{\omega \Delta t}{2}(p_n + p_{n+1})$$
$$p_{n+1} = p_n - \frac{\omega \Delta t}{2}(q_n + q_{n+1})$$

$$\begin{bmatrix} q_{n+1} \\ p_{n+1} \end{bmatrix} = \frac{1}{1 + \left(\frac{\omega \Delta t}{2}\right)^2} \begin{bmatrix} 1 - \left(\frac{\omega \Delta t}{2}\right)^2 & \omega \Delta t \\ -\omega \Delta t & 1 - \left(\frac{\omega \Delta t}{2}\right)^2 \end{bmatrix} \begin{bmatrix} q_n \\ p_n \end{bmatrix}$$

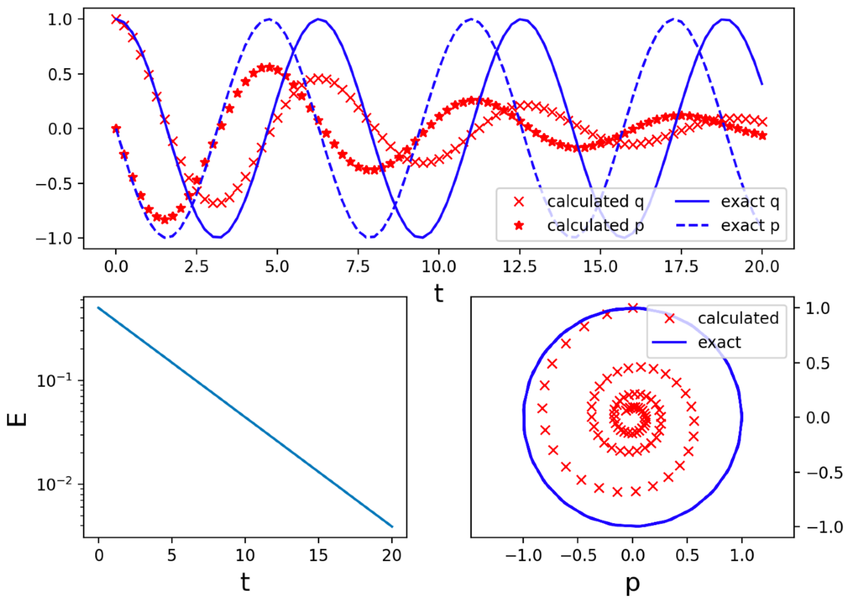
Stability analysis:

$$|\lambda_{1,2}| = 1$$

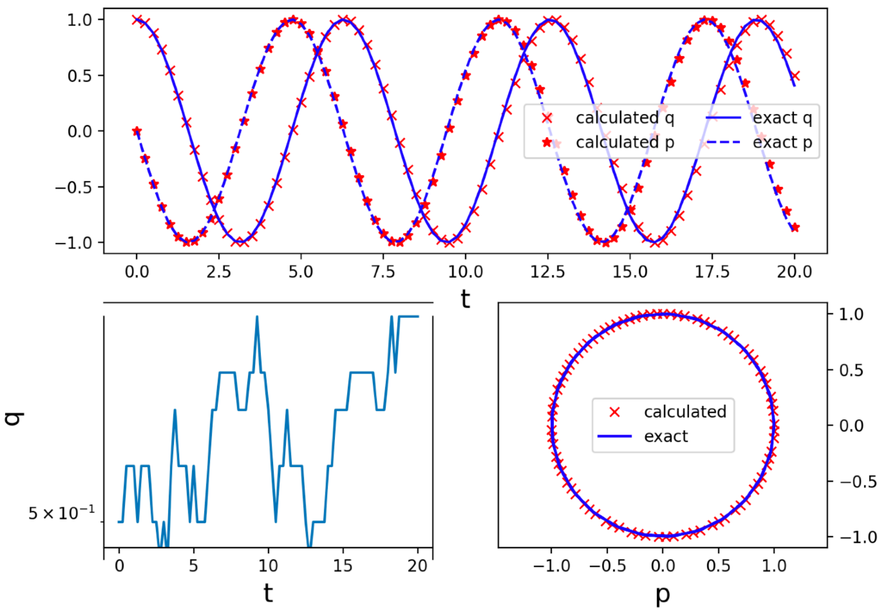
Q: DISCRETIZATION OF HARMONIC OSCILLATOR EQUATIONS

The three plots depict the evolution of the harmonic oscillator equations with ω=1, Δt= 0.25 for explicit, implicit and trapezoidal discretization. Associate the plots to the discretization

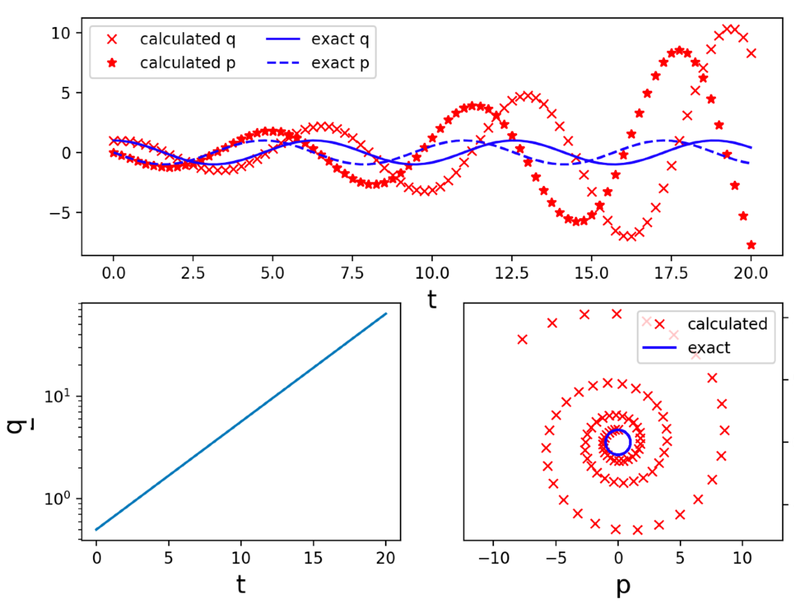
(a)



(b)



(c)



Q: DISCRETIZATION OF HARMONIC OSCILLATOR EQUATIONS

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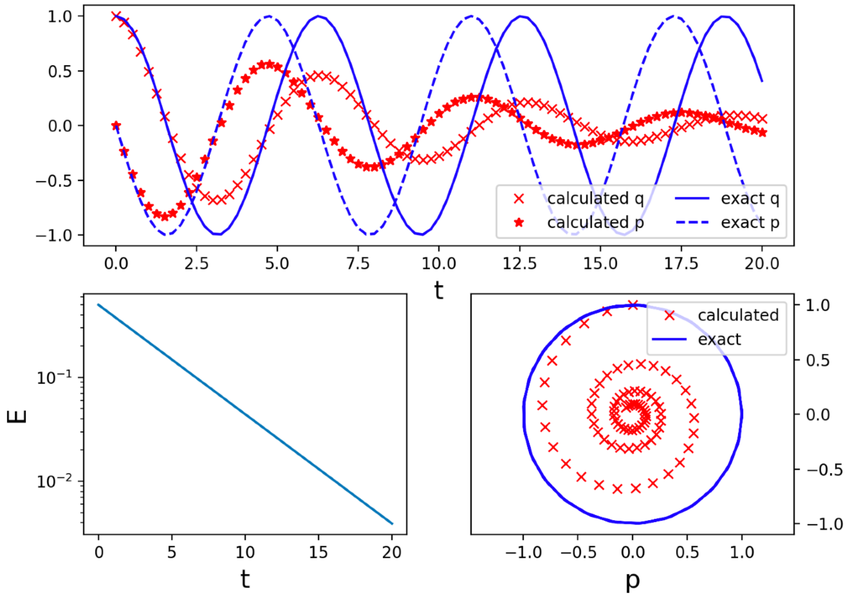
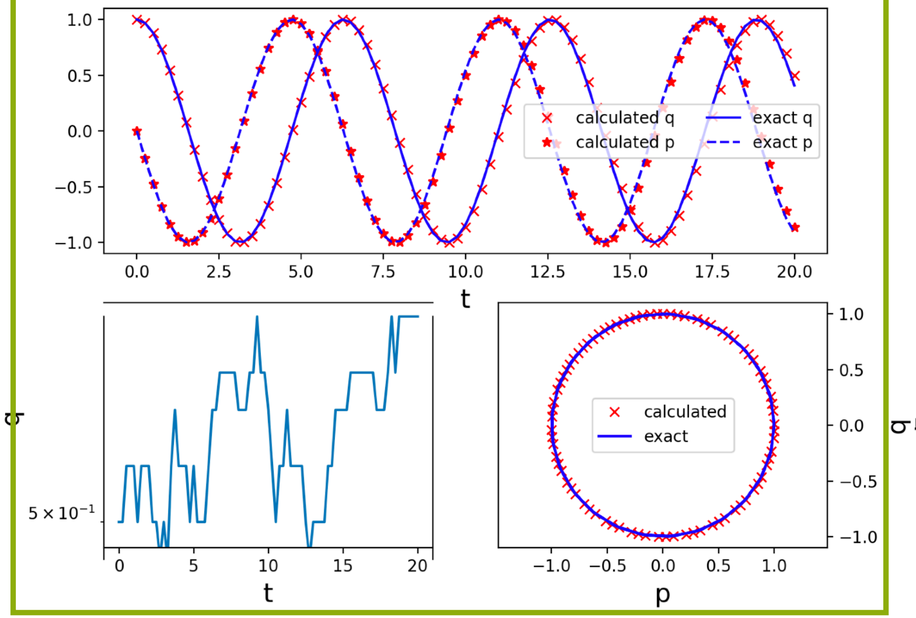
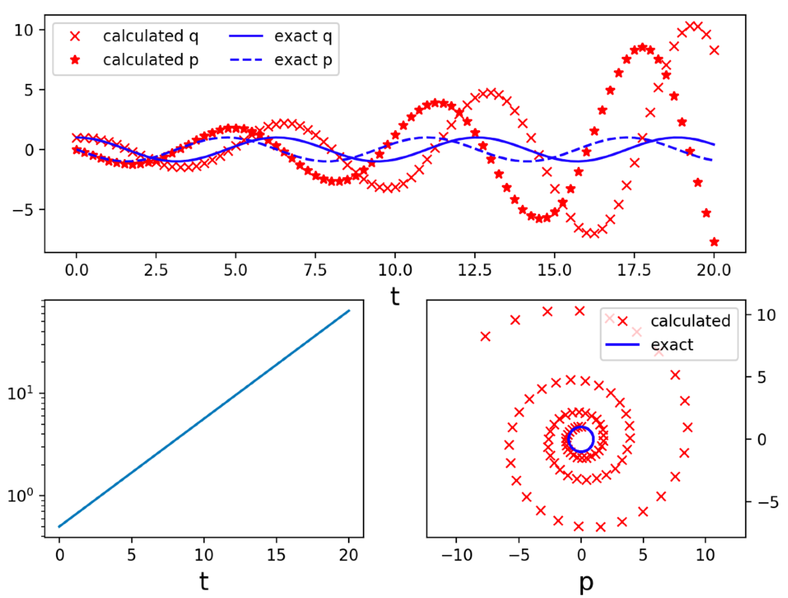
(a) Implicit



(b) Trapezoidal, θ=1/2



(c) Explicit



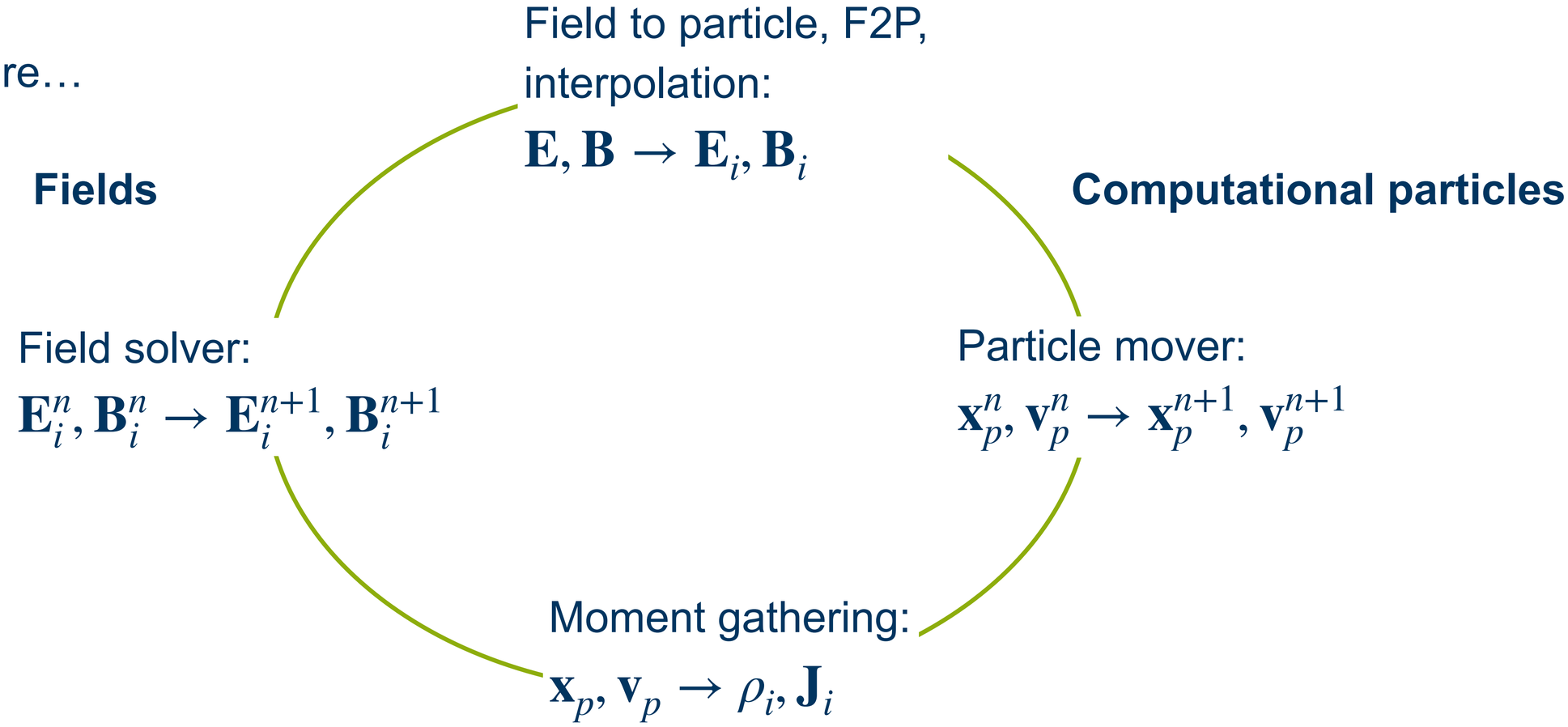
Advantage of evaluating the RHS at an intermediate time step

5. PIC METHODS & TEMPORAL DISCRETIZATION

TEMPORAL DISCRETIZATION IN PIC METHODS

Now we know the advantages of evaluating the RHS at an intermediate time step → let's see how it works out for PIC codes, ***for the coupled fields + particles system***

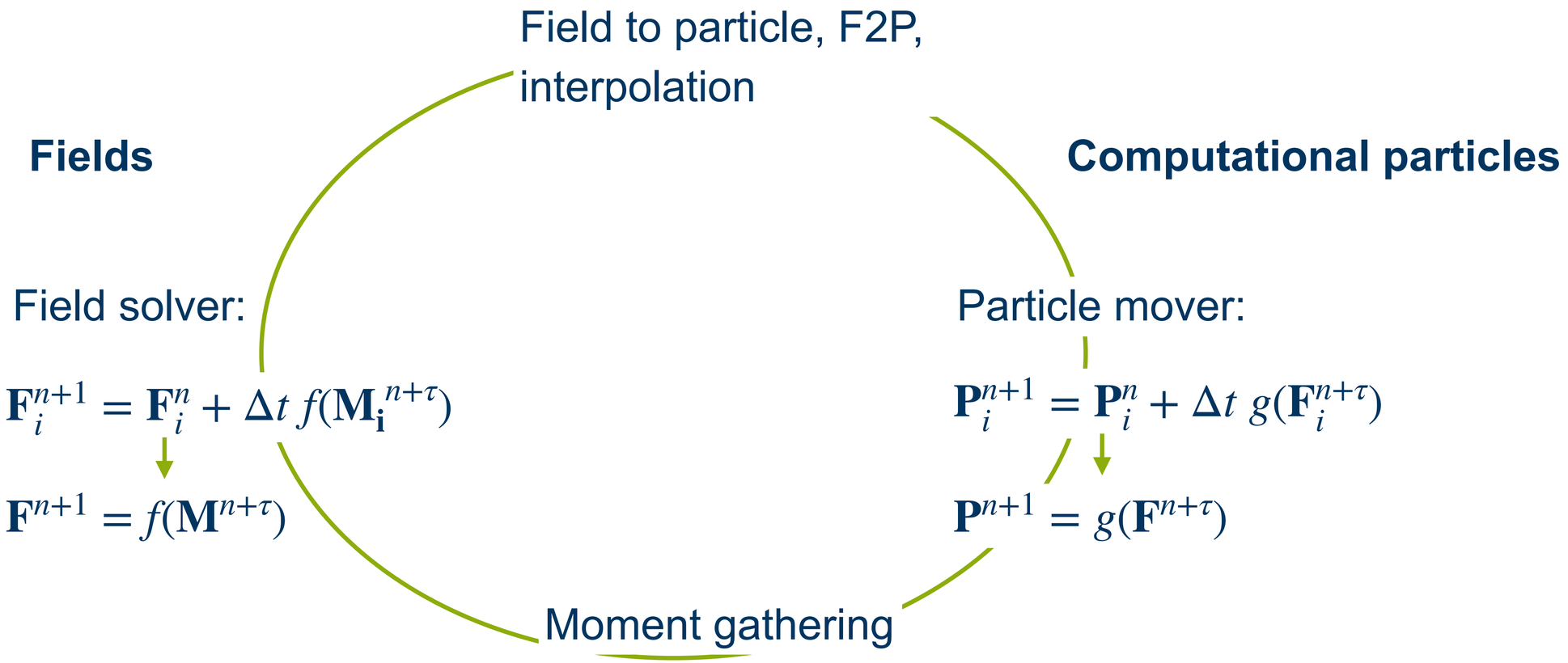
Where we were…



TEMPORAL DISCRETIZATION IN PIC METHODS

Let's change/ simplify the notation:

F: fields
P: particles
M: moments
τ> 0



Coupling between fields and particles!!!

EXPLICIT, SEMI-IMPLICIT AND IMPLICIT PIC CODES

$$\mathbf{F}^{n+1} = f(\mathbf{M}^{n+\tau}) \qquad \mathbf{P}^{n+1} = g(\mathbf{F}^{n+\tau})$$

Explicit

Hockney Eastwood 1990, Birdsall 2004

$$\mathbf{F}^{n+1} = f(\mathbf{M}^{n})$$
$$\mathbf{P}^{n+1} = g(\mathbf{F}^{n})$$

Stability constraints

$$c\Delta t < \Delta x$$
$$\Delta t \sim \omega_{pe}^{-1}$$
$$\Delta x \sim \lambda_D$$

Debye length

Semi-implicit

$$\mathbf{F}^{n+1} = f(\tilde{\mathbf{M}}^{n+\tau})$$
$$\mathbf{P}^{n+1} = g(\mathbf{F}^{n+1})$$

Direct Implicit
Cohen, 1989, Friedman, 1990, Hewett and Langdon, 1987, Tanaka, 1988, Gibbons and Hewitt, 1995

Implicit Moment Method
Mason 1987, Vu and Brackbill 1992, Lapenta 2006

Energy Conserving SI
Lapenta 2017

Stability constraints

$$\epsilon < v_{th,e}\frac{\Delta t}{\Delta x} < 1$$

Electron thermal velocity

Fully implicit

$$\mathbf{F}^{n+1} = f(\mathbf{M}^{n+1})$$
$$\mathbf{P}^{n+1} = g(\mathbf{F}^{n+1})$$

Solved together,
Size: particle #

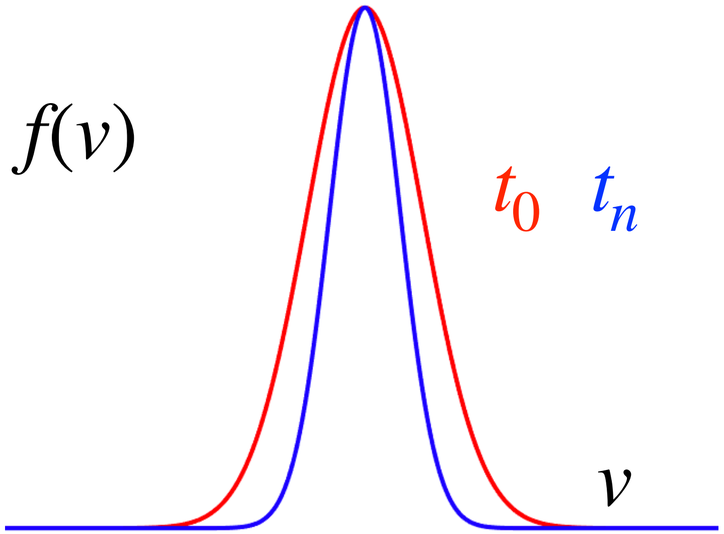
Chen Chacon 2011, Markidis Lapenta 2011

Stability constraints

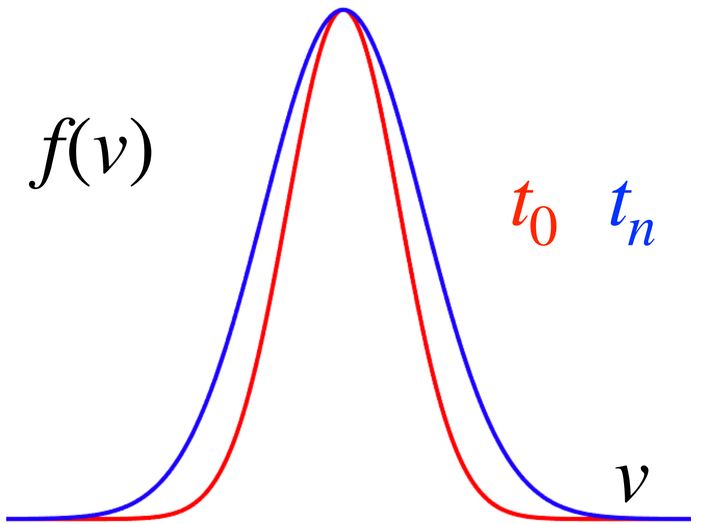
Effectively removed

Q: DISCRETIZATION AND EVOLUTION OF PARTICLE DISTRIBUTION FUNC.

Assume that the red curve is the electron velocity distribution function of a system at initialization. The same system is then evolved with either an explicit or (semi)-implicit PIC code, neither of them energy conserving. Associate the plot with the discretization



(a)



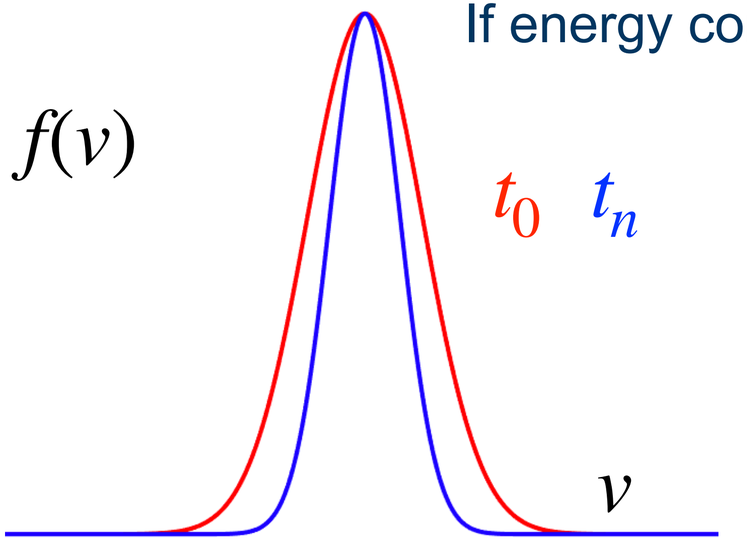
(b)

Q: DISCRETIZATION AND EVOLUTION OF PARTICLE DISTRIBUTION FUNC.

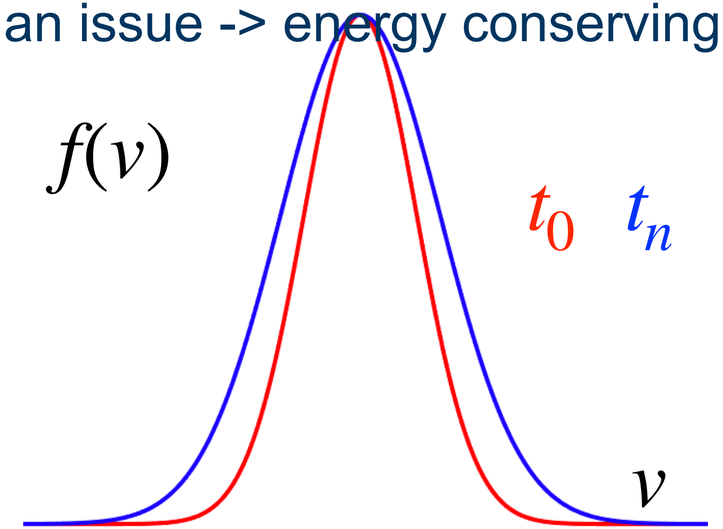
Assume that the red curve is the electron velocity distribution function of a system at initialization. The same system is then evolved with either an explicit or (semi)-implicit PIC code, neither of them energy conserving. Associate the plot with the discretization

heating/ cooling can be controlled with the choice of Δt/ θ; in explicit PIC we expect **numerical heating**, in implicit **numerical cooling**

If energy conservation is an issue -> energy conserving PICs



(a) implicit



(b) explicit

6. AN EXAMPLE OF SEMI-IMPLICIT DISCRETIZATION:

THE IMPLICIT MOMENT METHOD

THE IMPLICIT MOMENT METHOD

The Implicit Moment Method (Vu & Brackbill, 1982; Lapenta 2006) is an example of semi-implicit method. The stability constraint of explicit PIC codes is relaxed, at the price of moderately higher algorithmic complexity

Steps to derive the IMM

1. Semi- implicit discretisation of particle motion
2. Derivation of the equation for $E^{n+\theta}$, with particle sources at time $n+\theta$
3. **Approximation of particle sources**
4. Derivation of the equation for $E^{n+\theta}$, with approximated particle sources

The IMM is implemented in the C++, MPI code **iPic3D [Markidis et al, 2010]**

IMM: SEMI-IMPLICIT DISCRETIZATION OF PARTICLE MOTION/ 1

Discretisation of Newton's equations (Predictor- Corrector Crank Nicholson):

$$\mathbf{x}_p^{n+1} = \mathbf{x}_p^n + \bar{\mathbf{v}}_p \Delta t \qquad (1)$$

$$\mathbf{v}_p^{n+1} = \mathbf{v}_p^n + \frac{q_p \Delta t}{m_p}\left(\mathbf{E}_p^{n+\theta}\left(\bar{\mathbf{x}}_p\right) + \frac{\bar{\mathbf{v}}_p \times \mathbf{B}_p^n\left(\bar{\mathbf{x}}_p\right)}{c}\right) \qquad (2)$$

= @ future time, unknown by now

$\bar{\mathbf{x}}_p$ intermediate position: position at time n+1/2

$\bar{\mathbf{v}}_p$ intermediate velocity: velocity at time n+1/2

fields interpolated at intermediate (unknown) particle position

$$\bar{\mathbf{v}}_p = \frac{\mathbf{v}_p^{n+1} + \mathbf{v}_p^n}{2} \qquad (3)$$

Inserting (2) into (3)

$$\bar{\mathbf{v}}_p = \mathbf{v}_p^n + \frac{q_p \Delta t}{2 m_p}\left(\mathbf{E}_p^{n+\theta} + \frac{\bar{\mathbf{v}}_p \times \mathbf{B}_p^n}{c}\right) \qquad (4)$$

By taking (4) x $\mathbf{B}_p^n$ and using the vector identity (5):

$$\left(\bar{\mathbf{v}}_p \times \mathbf{B}_p^n\right) \times \mathbf{B}_p^n = -\bar{\mathbf{v}}_p \left|B_p^n\right|^2 + \left(\bar{\mathbf{v}}_p \cdot \mathbf{B}_p^n\right) \cdot \mathbf{B}_p^n \qquad (5)$$

IMM: SEMI-IMPLICIT DISCRETIZATION OF PARTICLE MOTION/ 2

we get

$$\bar{\mathbf{v}}_p \times \mathbf{B}_p^n = \mathbf{v}_p^n \times \mathbf{B}_p^n + \frac{q_p \Delta t}{2m_p}\left(\mathbf{E}_p^{n+\theta} \times \mathbf{B}_p^n + \frac{\left(\bar{\mathbf{v}}_p \cdot \mathbf{B}_p^n\right)}{c}\mathbf{B}_p^n - \frac{\bar{\mathbf{v}}_p \left|B_p^n\right|^2}{c}\right) \qquad (6)$$

Computing $\left(\bar{\mathbf{v}}_p \cdot \mathbf{B}_p^n\right)$ from (4)

$$\bar{\mathbf{v}}_p \times \mathbf{B}_p^n = \mathbf{v}_p^n \times \mathbf{B}_p^n + \frac{q_p \Delta t}{2m_p}\left(\mathbf{E}_p^{n+\theta} \times \mathbf{B}_p^n + \frac{\mathbf{v}_p^n \cdot \mathbf{B}_p^n}{c}\mathbf{B}_p^n + \right.$$

$$\left. + \frac{q_p \Delta t}{2m_p c}\left(\mathbf{E}_p^{n+\theta} \cdot \mathbf{B}_p^n\right)\mathbf{B}_p^n - \frac{\bar{\mathbf{v}}_p \left|B_p^n\right|^2}{c}\right) \qquad (7)$$

and inserting it into (4), defining $\hat{\mathbf{v}}_p$ as

$$\hat{\mathbf{v}}_p = \mathbf{v}_p^n + \frac{q_p \Delta t}{2m_p}\mathbf{E}_p^{n+\theta} \qquad (8)$$

we get a formula for the intermediate velocity:

$$\bar{\mathbf{v}}_p = \frac{\hat{\mathbf{v}}_p + \frac{q_p \Delta t}{2m_p c}\left(\hat{\mathbf{v}}_p \times \mathbf{B}_p^n + \frac{q_p \Delta t}{2m_p c}\left(\hat{\mathbf{v}}_p \cdot \mathbf{B}_p^n\right)\mathbf{B}_p^n\right)}{1 + \frac{q_p^2 \Delta t^2}{4m_p^2 c^2}\left|B_p^n\right|^2} \qquad (9)$$

Eq. for the intermediate velocity as a function of the electric field @ n+θ
BUT E and B are interpolated at the *intermediate* particle position

IMM: SEMI-IMPLICIT DISCRETIZATION OF PARTICLE MOTION/ 3

The mover is *iterative* (predictor corrector). The value of $\bar{\mathbf{v}}_p$ "improves" at every iteration k, and is finally used to calculate particle position and velocity at time t=n+1

$t = t^n$

$\bar{\mathbf{x}}_p^0 = \mathbf{x}_p^n$

k=0 $\quad \mathbf{E}_p^{n+\theta}\left(\bar{\mathbf{x}}_p^0\right)$, $\mathbf{B}_p^n\left(\bar{\mathbf{x}}_p^0\right)$ $\xrightarrow{(9)}$ $\bar{\mathbf{v}}_{\mathbf{p}}^0 \longrightarrow \bar{\mathbf{x}}_p^1 = \mathbf{x}_p^n + 1/2\bar{\mathbf{v}}_p^0 \Delta t$

k=1 $\quad \mathbf{E}_p^{n+\theta}\left(\bar{\mathbf{x}}_p^1\right)$, $\mathbf{B}_p^n\left(\bar{\mathbf{x}}_p^1\right)$ $\xrightarrow{(9)}$ $\bar{\mathbf{v}}_{\mathbf{p}}^1 \longrightarrow \bar{\mathbf{x}}_p^2 = \mathbf{x}_p^n + 1/2\bar{\mathbf{v}}_p^1 \Delta t$

$t = t^{n+1}$

k=K

$$\mathbf{v}_p^{n+1} = 2\bar{\mathbf{v}}_p^k - \mathbf{v}_p^n$$

$$\mathbf{x}_p^{n+1} = \mathbf{x}_p^n + \bar{\mathbf{v}}_p^k \Delta t$$

but we still need to know $E^{n+\theta}$ to calculate the intermediate velocity, so we need a formula for $E^{n+\theta} = f(x^n, v^n)$ first

IMM: DERIVATION OF THE EQUATION FOR $E^{n+\theta}$, WITH PARTICLE SOURCES AT TIME n+θ

Semi-implicit discretisation of Faraday's and Ampere's equations:

$$\mathbf{B}^{n+1} = \mathbf{B}^n - c\Delta t \nabla \times \mathbf{E}^{n+\theta} \qquad (1)$$

$$\mathbf{E}^{n+1} = \mathbf{E}^n + c\Delta t \left(\nabla \times \mathbf{B}^{n+\theta} - \frac{4\pi}{c} \mathbf{J}^{n+\theta} \right) \qquad (2)$$

= @ future time, unknown by now

To obtain $\nabla \times \mathbf{B}^{n+\theta}$: curl of (1), vector identity (3), time-discretised Gauss' law (4), (5)

$$\nabla \times \left(\nabla \times \mathbf{E}^{n+\theta} \right) = \nabla \cdot \left(\nabla \cdot \mathbf{E}^{n+\theta} \right) - \nabla^2 \mathbf{E}^{n+\theta} \qquad (3)$$

$$\nabla \cdot \mathbf{E}^{n+\theta} = 4\pi \rho^{n+\theta} \qquad (4)$$

$$\nabla \times \mathbf{B}^{n+\theta} = (1-\theta) \nabla \times \mathbf{B}^n + \theta \nabla \times \mathbf{B}^{n+1} \qquad (5)$$

$$\longrightarrow \quad \nabla \times \mathbf{B}^{n+\theta} = \nabla \times \mathbf{B}^n + c\theta\Delta t \left(\nabla^2 \mathbf{E}^{n+\theta} - \nabla \cdot 4\pi \rho^{n+\theta} \right) \quad \text{, back in (2)}$$

$$\mathbf{E}^{n+\theta} - (c\theta\Delta t)^2 \nabla^2 \mathbf{E}^{n+\theta} = \qquad (6)$$

$$\mathbf{E}^n + c\theta\Delta t \left(\nabla \times \mathbf{B}^n - \frac{4\pi}{c} \mathbf{J}^{n+\theta} \right) - (c\theta\Delta t)^2 4\pi \nabla \rho^{n+\theta}$$

Eq. for E @ n+θ BUT our sources are also at advanced time

WHERE WE ARE NOW

Equations for particle motion: still need $\mathbf{E}_p^{n+\theta}$

$$\mathbf{x}_p^{n+1} = \mathbf{x}_p^n + \bar{\mathbf{v}}_p \Delta t$$

$$\mathbf{v}_p^{n+1} = \mathbf{v}_p^n + \frac{q_p \Delta t}{m_p} \left(\mathbf{E}_p^{n+\theta}\left(\bar{\mathbf{x}}_p\right) + \frac{\bar{\mathbf{v}}_p \times \mathbf{B}_p^n\left(\bar{\mathbf{x}}_p\right)}{c} \right)$$

$$\bar{\mathbf{v}}_p = \frac{\hat{\mathbf{v}}_p + \frac{q_p \Delta t}{2 m_p c} \left(\hat{\mathbf{v}}_p \times \mathbf{B}_p^n + \frac{q_p \Delta t}{2 m_p c} \left(\hat{\mathbf{v}}_p \cdot \mathbf{B}_p^n \right) \mathbf{B}_p^n \right)}{1 + \frac{q_p^2 \Delta t^2}{4 m_p^2 c^2} \left| B_p^n \right|^2}$$

$$\hat{\mathbf{v}}_p = \mathbf{v}_p^n + \frac{q_p \Delta t}{2 m_p} \mathbf{E}_p^{n+\theta}$$

Equations for field update: still need advanced moments, $\mathbf{J}^{n+\theta}$, $\rho^{n+\theta}$

$$\mathbf{E}^{n+\theta} - \left(c\theta\Delta t\right)^2 \nabla^2 \mathbf{E}^{n+\theta} =$$
$$\mathbf{E}^n + c\theta\Delta t \left(\nabla \times \mathbf{B}^n - \frac{4\pi}{c} \mathbf{J}^{n+\theta} \right) - \left(c\theta\Delta t\right)^2 4\pi \nabla \rho^{n+\theta}$$

IMM: APPROXIMATION OF PARTICLE SOURCES

Now we need to express $\rho^{n+\theta}$ and $\mathbf{J}^{n+\theta}$n terms of something we can work with:
let's approximate them around the particle position at *time step n*

$$f(y) \sim f(a) + f'(a)(y-a) + 1/2 f''(a)(y-a)^2 + ...$$

$$y = x - x^{n+\theta}$$

$$a = x - x^{n}$$

Taylor expansion of f(y) around y=a

Here:

$$\rho^{n+\theta} = \sum_p q_p S(\mathbf{x} - \mathbf{x}^{n+\theta}) \sim \sum_p q_p \left[S(\mathbf{x} - \mathbf{x}^n) - (\mathbf{x}^{n+\theta} - \mathbf{x}^n) \nabla \cdot S(\mathbf{x} - \mathbf{x}^n) + ... \right] \quad (1)$$

Equivalent at the II order to

Heuristic explanation for stability constraint: the *average* electron cannot move more than a Dx in a Dt

$$\rho^{n+\theta} \sim \sum_p q_p \left[S(\mathbf{x} - \mathbf{x}^n) - \underbrace{(\mathbf{x}^{n+\theta} - \mathbf{x}^n)}_{-\theta \Delta t \bar{\mathbf{v}}_p} \nabla \cdot S(\mathbf{x} - \mathbf{x}^{n+\theta}) \right] =$$

$$\rho^n - \theta \Delta t \nabla \cdot \underbrace{\sum_p q_p \bar{\mathbf{v}}_p S(\mathbf{x} - \mathbf{x}^{n+\theta})}_{\mathbf{J}^{n+\theta}} = \rho^n - \theta \Delta t \nabla \cdot \mathbf{J}^{n+\theta} \quad (2)$$

IMM: APPROXIMATION OF PARTICLE SOURCES/ 2

We can use the same approximation for $\mathbf{J}^{n+\theta}$

$$\mathbf{J}^{n+\theta} = \sum_p q_p \bar{\mathbf{v}}_p S(\mathbf{x} - \mathbf{x}^n) - \theta \Delta t \nabla \cdot \sum_p q_p \bar{\mathbf{v}}_p \bar{\mathbf{v}}_p S(\mathbf{x} - \mathbf{x}^n) \qquad (3)$$

which, rewriting (9) as

$$\bar{\mathbf{v}}_p = \tilde{\mathbf{v}}_p + \beta_p \tilde{\mathbf{E}}^{n+\theta} \qquad \beta_p = \frac{q_p \Delta t}{2 m_p} \qquad \mu_\cdot = \sum_s \mu_{s\cdot}$$

$$\tilde{\mathbf{v}}_p = \mathbf{R}_p \cdot \mathbf{v}_p \qquad \tilde{\mathbf{E}}_p^{n+\theta} = \mathbf{R}_p \cdot \mathbf{E}^{n+\theta} \qquad \mu_{s\cdot} = 4\pi\theta\Delta t \beta_s \rho_s \sum_p \mathbf{R}_p$$

$$\mathbf{R}_{p\cdot} = \frac{\mathbf{I} - \frac{\beta_p}{c}\mathbf{I} \times \mathbf{B}_p^n + \frac{\beta_p^2}{c^2}\mathbf{B}_p^n \cdot \mathbf{B}_p^n}{1 + \frac{\beta_p^2}{c^2}\left|B_p^n\right|^2}.$$

and with $\hat{\mathbf{J}}^n = \sum_p q_p \tilde{\mathbf{v}}_p S(\mathbf{x} - \mathbf{x}^n) - \theta \Delta t \nabla \cdot \sum_p q_p \tilde{\mathbf{v}}_p \tilde{\mathbf{v}}_p S(\mathbf{x} - \mathbf{x}^n)$ (4)

gives $\mathbf{J}^{n+\theta} = \hat{\mathbf{J}}^n + \frac{1}{4\pi\theta\Delta t}\mu \cdot \mathbf{E}^{n+\theta}$ (5)

now we can express the time-advanced moments as $f(x^n, v^n, B^n)+g(E^{n+\theta})$

IMM: DERIVATION OF THE EQUATION FOR $E^{n+\theta}$, WITH APPROXIMATED PARTICLE SOURCES

Inserting (2) and (5) into (6) and with

$$\hat{\rho}^n = \rho^n - \Delta t \theta \nabla \cdot \hat{\mathbf{J}}^n$$

we finally get a formula for $E^{n+\theta}$ only in terms of known quantities:

Now everything in the RHS is known!

$$(\mathbf{I} + \mu) \cdot \mathbf{E}^{n+\theta} - (c\theta\Delta t)^2 \left(\nabla^2 \mathbf{E}^{n+\theta} + \nabla\nabla \cdot \left(\mu \cdot \mathbf{E}^{n+\theta} \right) \right) =$$
$$\mathbf{E}^n + c\theta\Delta t \left(\nabla \times \mathbf{B}^n - \frac{4\pi}{c} \hat{\mathbf{J}}^n \right) - (c\theta\Delta t)^2 4\pi \nabla \hat{\rho}^n$$

This is an equation of the type AX=B which can be solved with a GMRES (Generalized Minimal RESidual method) solver [Saad 2003].

B^{n+1} is then obtained from (1)

HOW TO CHOOSE Θ?

- ✓ $1/2 \leq \theta \leq 1$
- ✓ $\theta = 1/2$: second order in time; otherwise, first order
- ✓ larger θ, more “implicit”: higher degree of numerical cooling
- ✓ as a rule of thumb, the lower the resolution (ion scale resolution), the larger the θ: we need to damp more the unresolved frequencies/ wavenumbers
- ✓ convergence studies are important!

7. SEMI-IMPLICIT PIC AS A BRIDGE BETWEEN KINETIC AND LARGER SCALES

THE ONE THING FROM THIS LECTURE YOU DO NOT WANT TO FORGET

Core of semi-implicit PIC methods: the temporal discretization results in this stability constraint:

$$\epsilon < v_{th,e}\frac{\Delta t}{\Delta x} < 1$$

CFL condition on the average electron thermal velocity

What does this mean?

✓ The Δt, Δx that we can use are larger then with explicit PIC

+: simulations cost less, we can study problems otherwise inaccessible

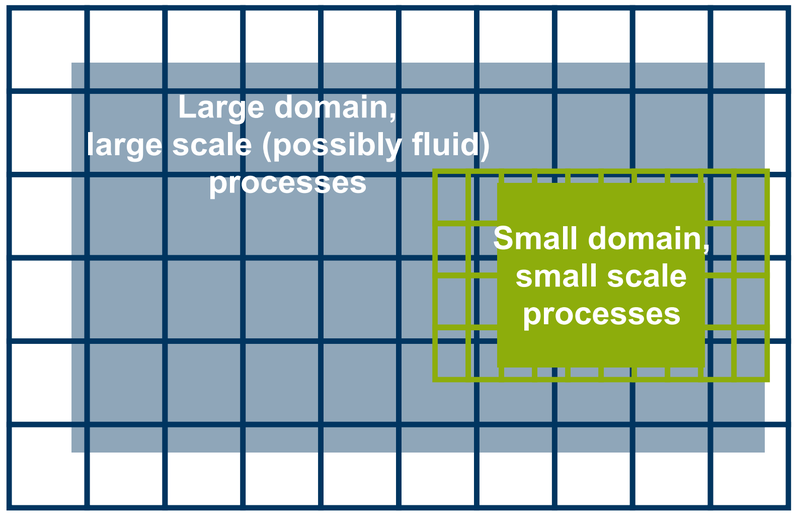
-: more thoughts has to go into choice of resolution: we have to resolve whatever we are interested in, convergence studies usually take longer

✓ We can get closer to “system” scales: **semi-implicit PIC are the kinetic method of choice for code coupling**

CODE COUPLING

Code coupling: coupling together different codes, or the same code used "differently" (e.g., different resolution) to focus on processes occurring at different scales in different parts of the simulation

(we are making here a somehow artificial difference between code coupling and Adaptive Mesh Refinement, AMR)



+: the computational cost of certain simulations is drastically reduced, we can study problems otherwise too expensive for kinetic codes

-: coupled code are trickier to develop and program, we have to be more careful of numerical artifacts

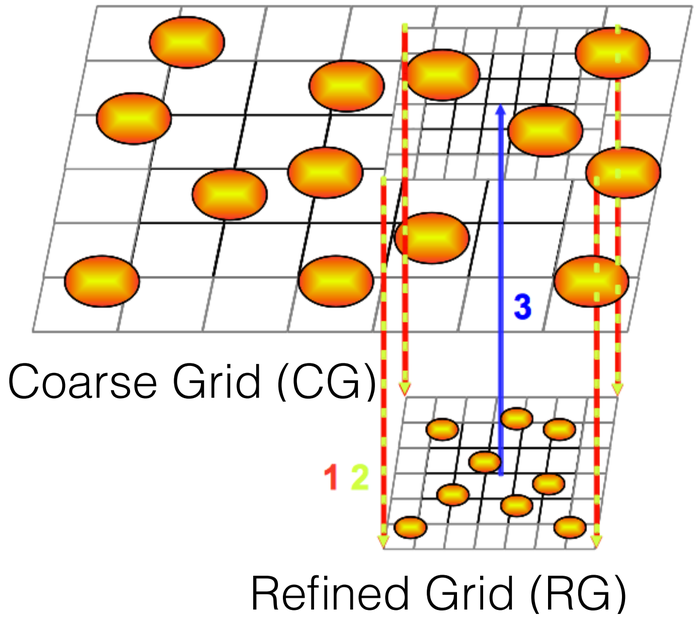
We focus on:

✓ kinetic/ kinetic coupling

✓ fluid/ kinetic coupling

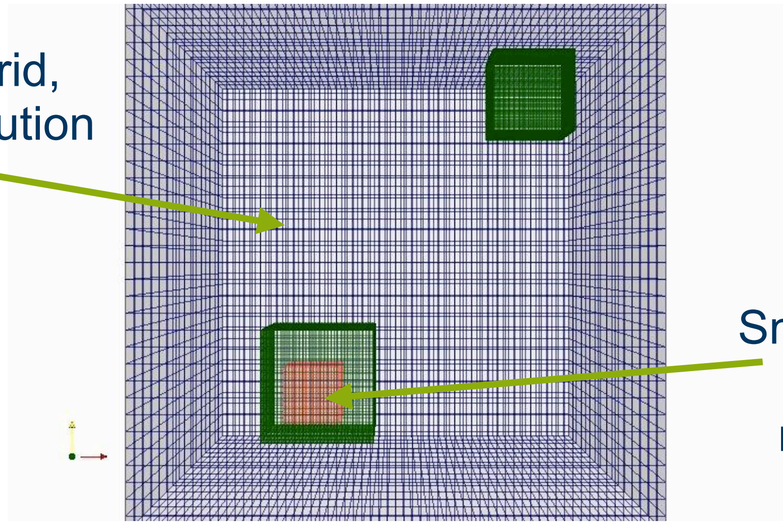
See **Simon Lautenbach**'s lecture tomorrow!

KINETIC/ KINETIC COUPLING: THE MULTI-LEVEL MULTI-DOMAIN METHOD



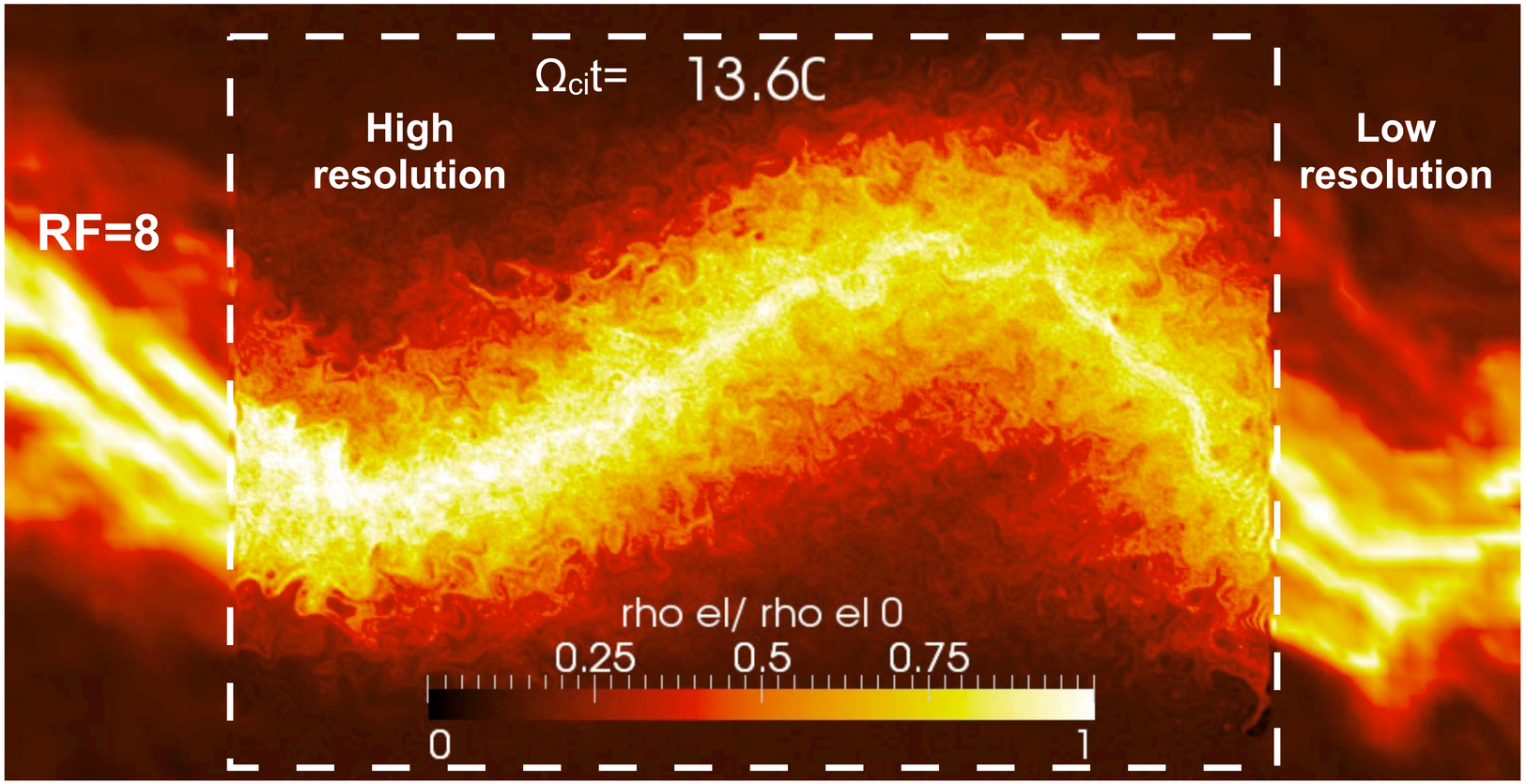
The MLMD method is a variation on the theme of Adaptive Mesh Refinement (AMR) PIC (e.g. Vay et al 2004, Fujimoto et al 2008).
In a MLMD system, different grids are resolved with an *IMM PIC at different resolution*. The Coarse Grid drives the evolution of the Refined Grid through field and particle Boundary Conditions
The method saves computational time w.r.t. resolving everything with the highest resolution

Large resolution jumps (e.g. ion scale resolution on a grid, electron scale on another) are made possible by the large stability region of the IMM.
Resolution jumps of 14 in space, 10 in time where reached **[Innocenti et al 2015]**



EXAMPLE OF MLMD SIMULATION

Lower Hybrid Drift Instability simulation



$m_i/m_e=1836$

$dx_{CG}= 0.078\ d_i$

$dx_{RF}= 0.42\ d_e$

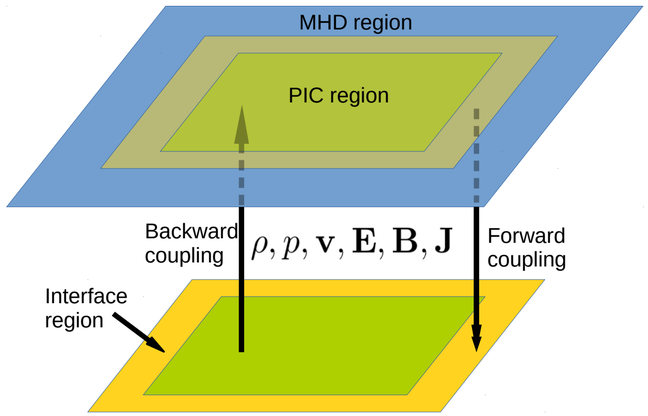
$dt_{CG}=0.1\ \omega_{pi}^{-1}$

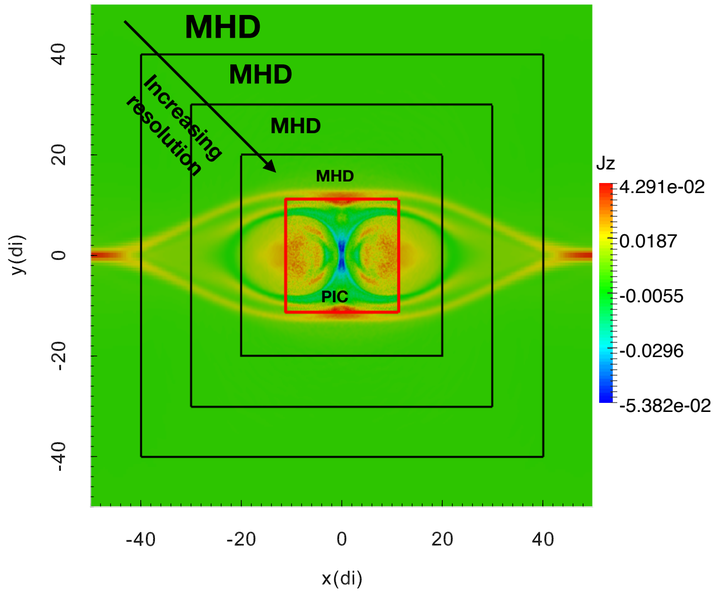
$dx_{CG}/dx_{RF}=8$

$dt_{CG}/dt_{RF}=2$

modified from **Innocenti et al 2016**

FLUID/ KINETIC COUPLING





In fluid-kinetic coupled codes, the challenge is not the different resolution, but the *different physical description*, MHD vs PIC

The MHD simulation is used to initialize the PIC simulation in an embedded region within the global MHD domain

In forward coupling, the MHD solution in the interface region is provided as boundary condition to the fields and particles of PIC at every time step

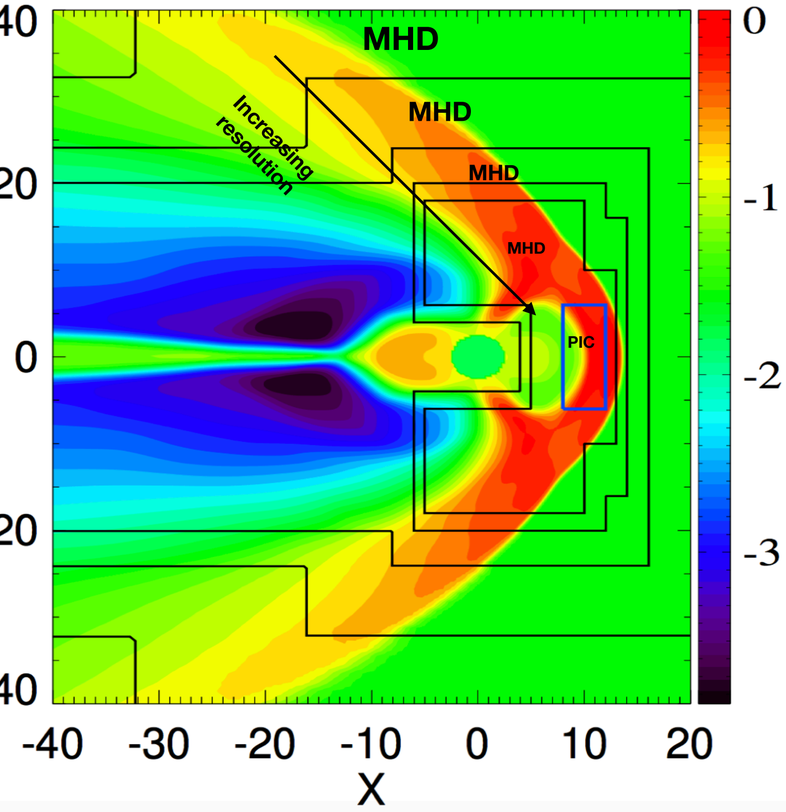
In backward coupling, the PIC moments are used to update the MHD solution after every time step

Several levels of grid refinement may be used to decrease the resolution of the MHD grid to match the one of the PIC mesh

Makwana et al 2017: AMR-VAC+ KUL iPic3D: Coalescence of current channels with 4 mesh levels in MHD (black boxes) and an embedded PIC region (red box) around the reconnection zone

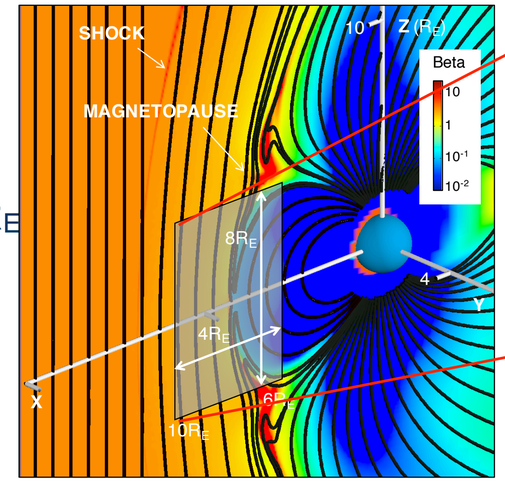
EXAMPLE OF FLUID/ KINETIC COUPLING

Aim: study kinetic processes embedded in large domains which cannot be simulated kinetically due to the large computational cost

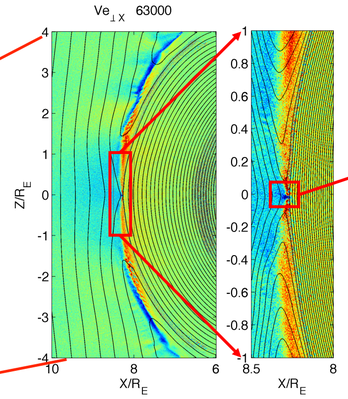


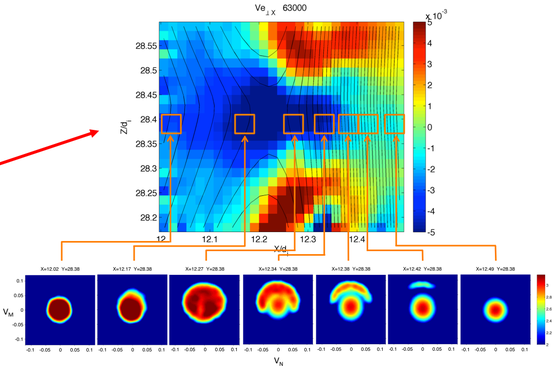
Chen et al 2017: BATS-R-US+ KTH iPic3D: MHD-EPIC 3D simulations of Earth's dayside reconnection to study Flux Transfer Events

PIC area:
8 R_E < x < 12 R_E
–6 R_E to 6 R_E,
–6 R_E < z < 6 R_E ,
dx/R_E =1/16



Berchem et al 2017: UCLA global MHD code+ KUL iPic3D: dayside reconnection, formation of electron crescent, as predicted numerically by Hesse 2014 and observed by MMS





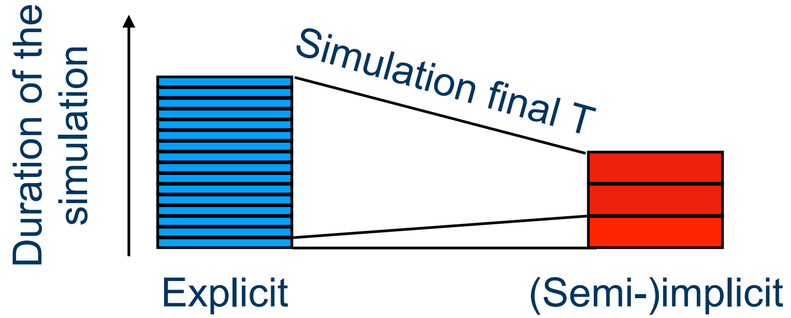
PIC area:
6 R_E < x < 10 R_E, = 28.5 d_i
−4 R_E < z < 4 R_E = 57 d_i
dx= 0.0178 d_i = 0.09 d_e

8. CLOSING CONSIDERATIONS

SEMI-IMPLICIT PIC METHODS

- ✓ Aim: save computational time w.r.t. explicit PIC via more lenient stability constraints
- ✓ How it works (in most s-i methods): particle sources in field equations at advanced times are approximated using available information at present time
- ✓ What happens: one step of a semi-implicit PIC code is heavier than explicit, it becomes convenient if less steps are needed to reach the final time due to larger Dt
- ✓ What it allows: fully kinetic simulations of larger domains, for longer times, with reduced approximations (e.g., larger mass ratio than explicit); code coupling become easier
- ✓ A word of caution: it's not magic, processes not resolved are simulated only qualitatively; convergence tests are even more crucial!

$$\epsilon < v_{th,e}\frac{\Delta t}{\Delta x} < 1$$



THANK YOU FOR YOUR ATTENTION!