Gyro-resolved nonlinear kinetic effects at topologically complex plasma-material interfaces

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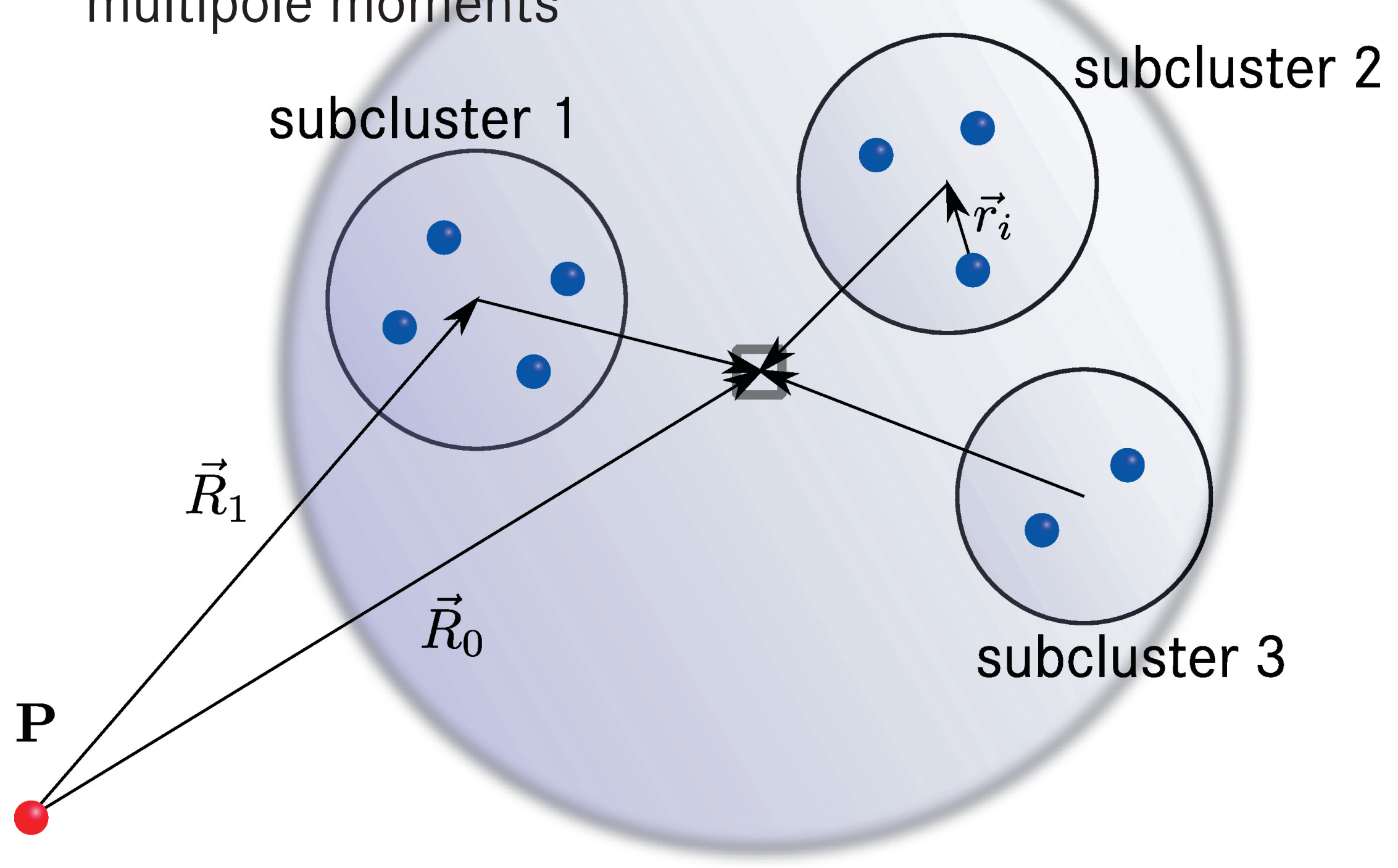
Barnes-Hut [1]

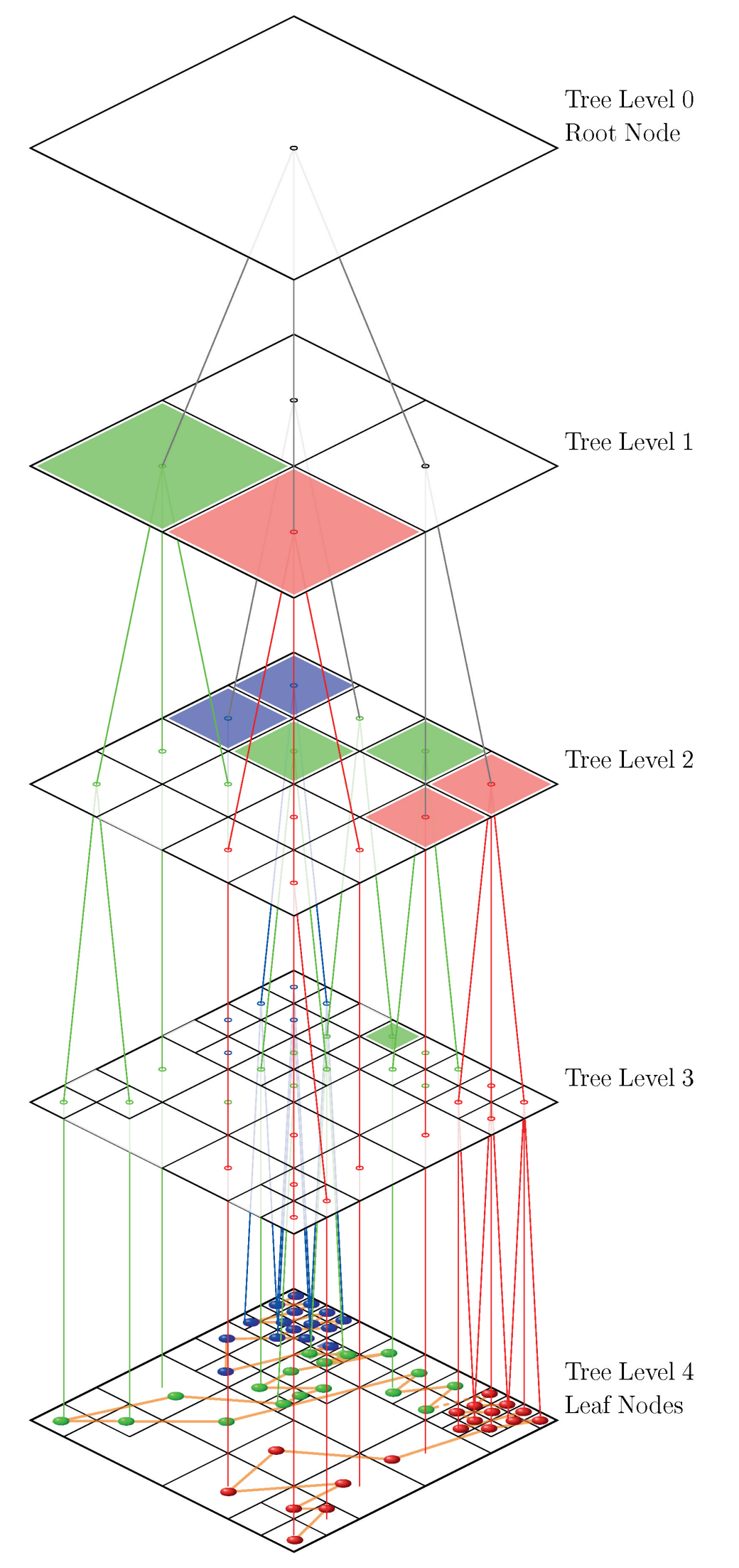
- solves electrostatics using Green's function

$$\Delta\,\Phi = \rho \quad \rightarrow \quad \Phi\,(x) = \sum_i q_i\, G\,(x, x_i)$$

- reduces complexity of *N*-body problems from *O(N²)* to *O(N log N)*
- charges combined into hierarchic groups of multipole moments



Algorithm phases [2]



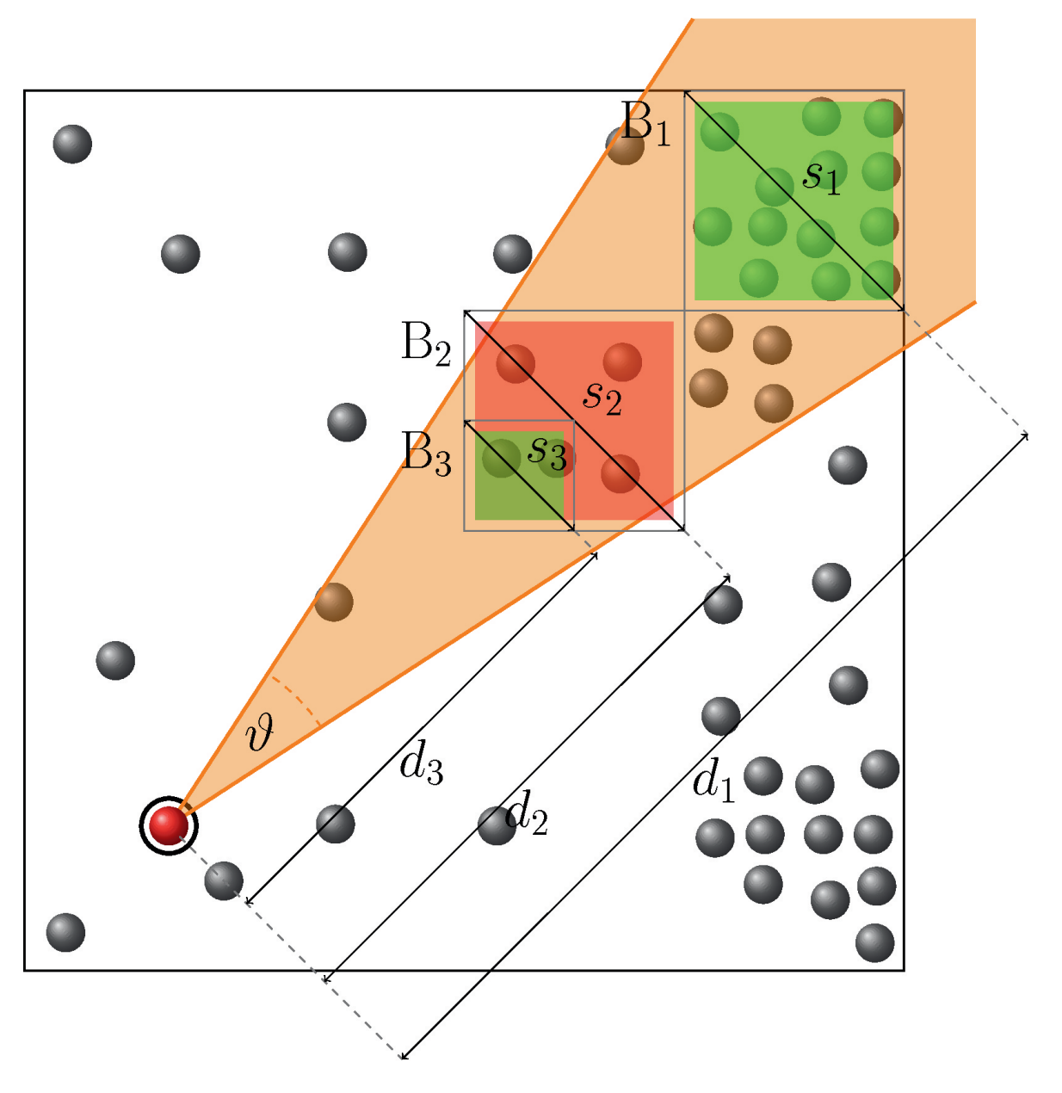
Input: Source positions & charges, sink positions

1. **Domain decomposition**
   - thread particles onto a space-filling curve (Morton, Hilbert, ...)
   - redistribute particles on parallel processors
2. **Tree construction**
   - compute multipole moments at lowest level and propagate upwards
   - identify and exchange branch nodes
   - construct global tree
3. **Tree traversal**
   - find interaction partners using a multipole acceptance criterion

$$\theta \geq \frac{s}{d}$$

   - gather remote sub-branch nodes if necessary
   - compute interactions

Output: Potential & electric field at sink positions

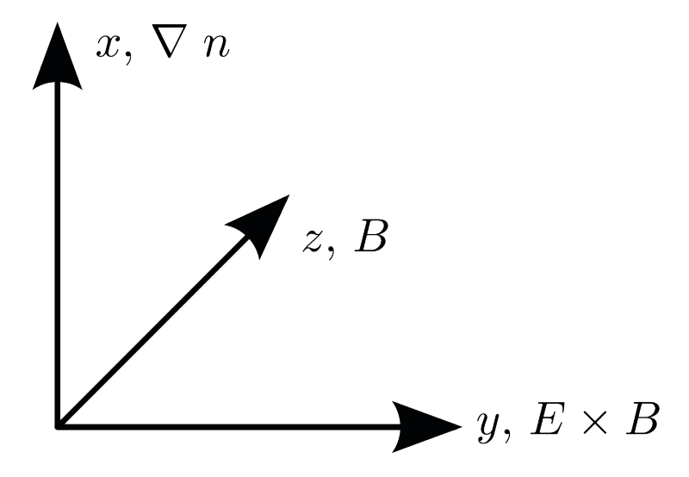


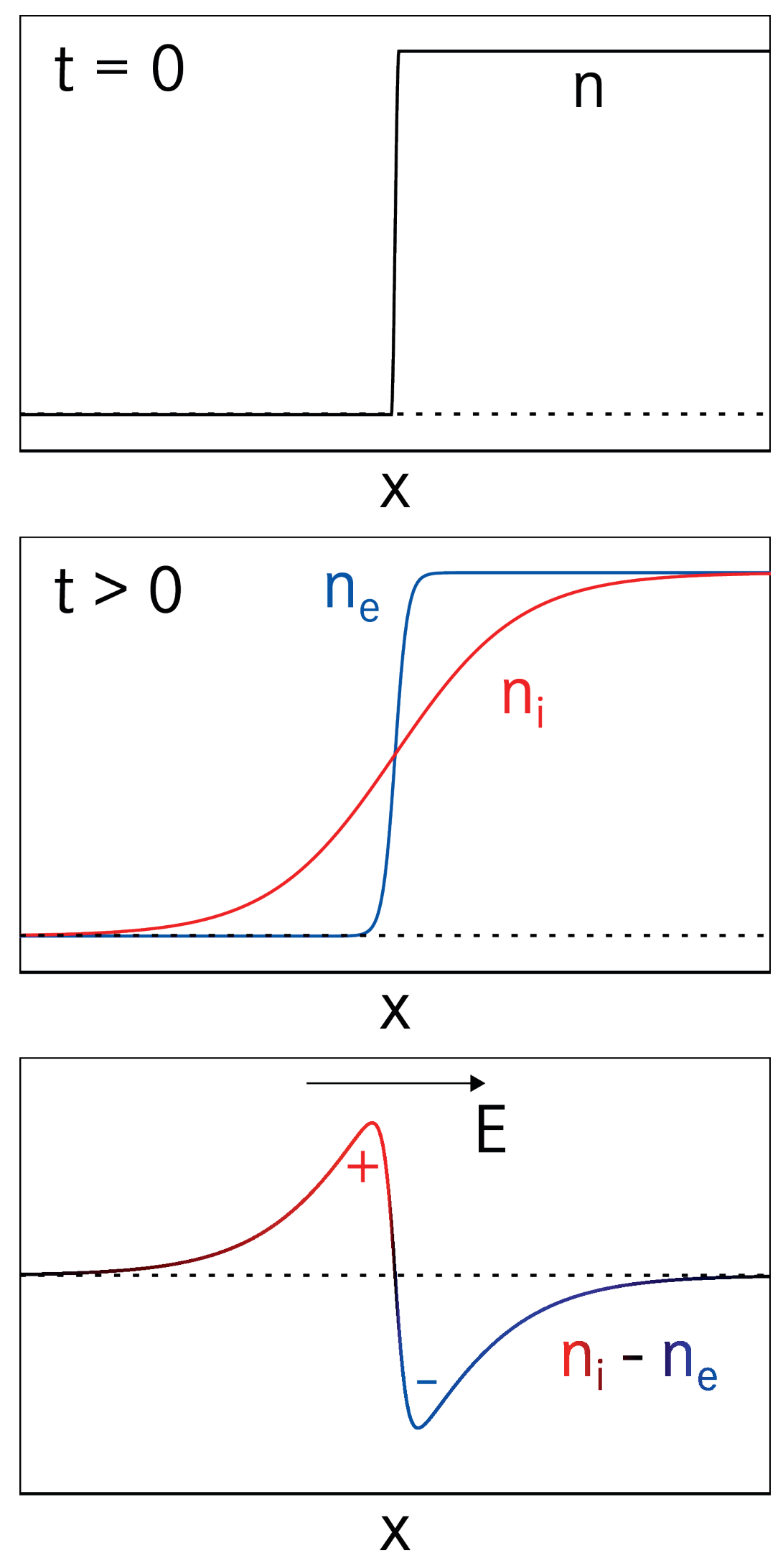
Kelvin-Helmholtz instabilities at plasma-vacuum interfaces

Driving mechanism

1. magnetised plasma slab, n = const., in contact with vacuum
2. different Larmor radii lead to different density gradient scales
3. charge separation creates a sheared electric field

sheared *E x B* flow feeds KH instability

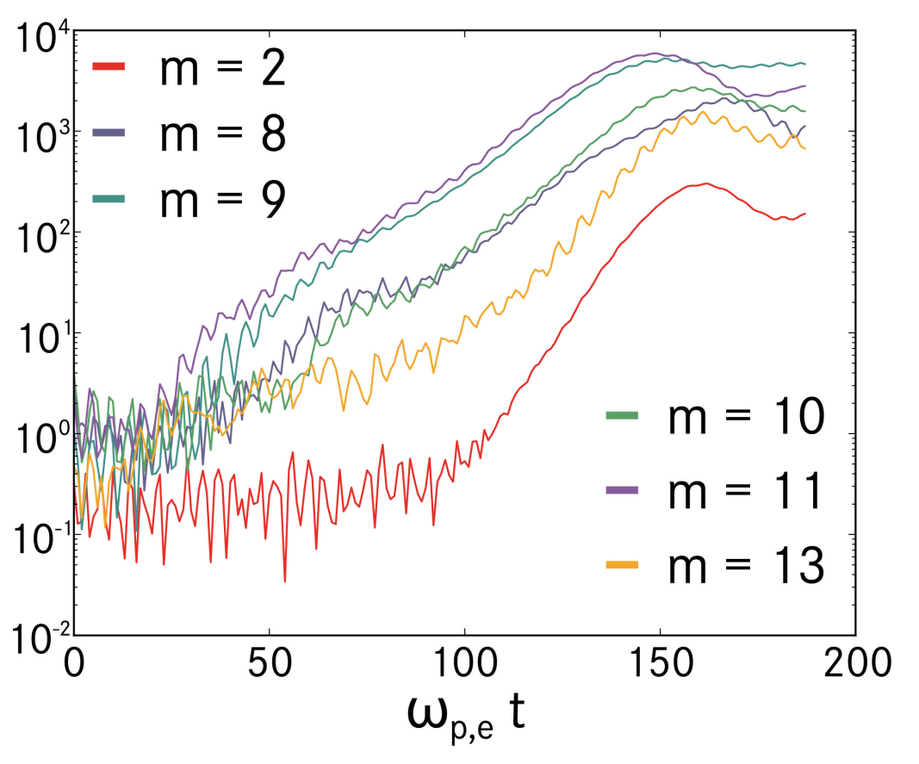


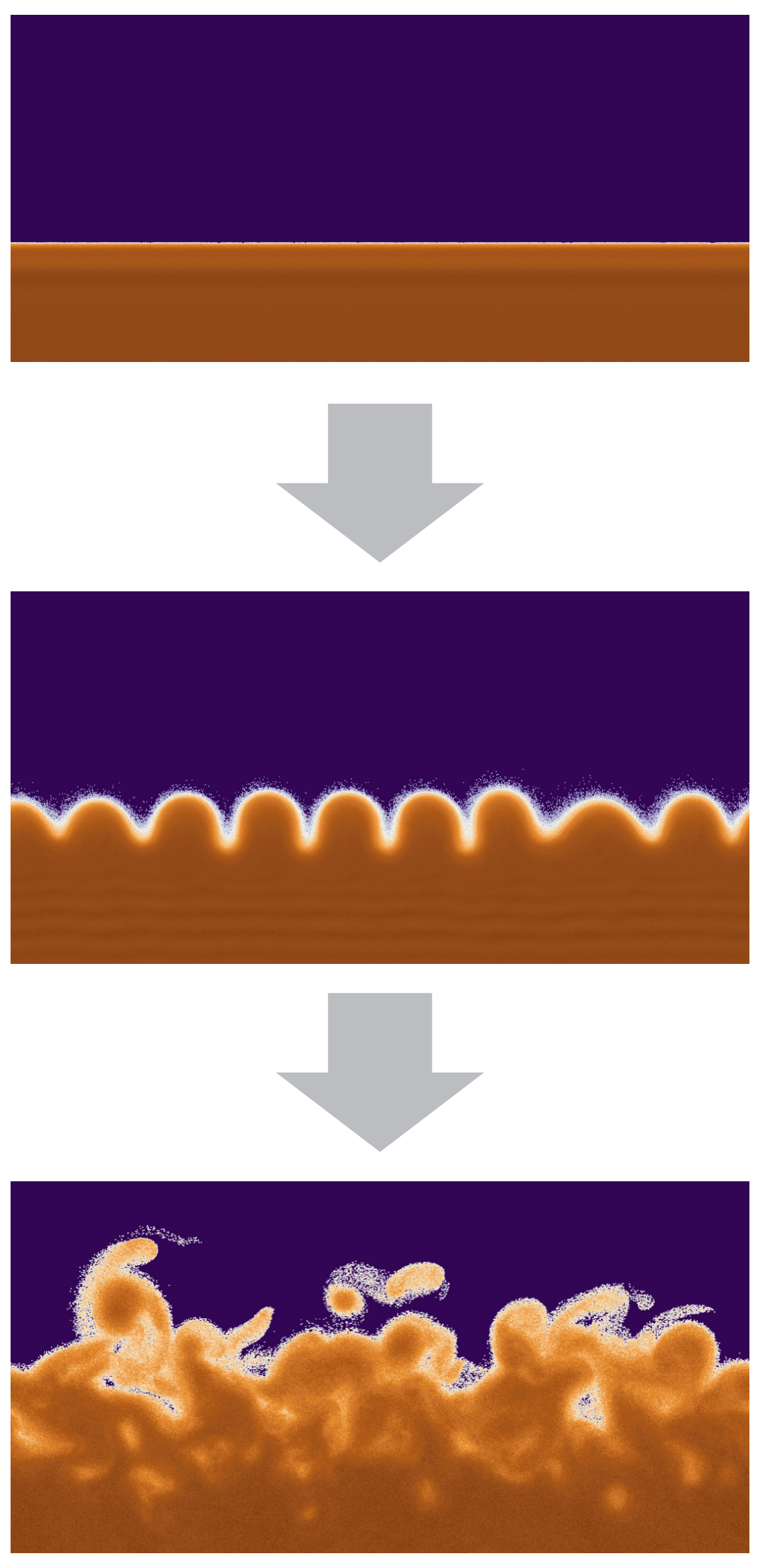


Evolution (right)

1. initial phase, homogeneous gradient
2. linear phase, exponentially growing perturbation
3. nonlinear phase, forming of vortex structures

Growth rates (below)





Parallel treecode PEPC [3]

- parallel Barnes-Hut algorithm implemented in treecode PEPC
- freely available for:
  - JUQUEEN (Blue Gene/Q, 458,752 cores)
  - JUROPA (Intel Nehalem, 17,664 cores)
  - GNU/Linux workstations
  - Mac OS X
- innovative hybrid parallelisation scheme using MPI and POSIX threads

- very promising scaling behaviour to reasonably utilise **up to 450,000 CPUs** running **1,600,000 threads** in simulations with **up to 65 billion particles**
- supports several interaction kernels: Coulomb 2D & 3D, vortex fluid dynamics, ...

Boundary Element Method (BEM) [4]

Electrostatics with boundary conditions:

$$\Phi(x) = \bar{\Phi}(x),\ \ x \in \partial\Omega_D \qquad \partial_n\Phi(x) = \bar{q}(x),\ \ x \in \partial\Omega_N$$

Green's function representation:

$$\Phi(x) = \underbrace{\ldots}_{\text{above}} + \int_{\partial\Omega} \left[\bar{\Phi}(x')\partial'_n G(x, x') - \bar{q}(x')G(x, x') \right] \mathrm{d}S'$$

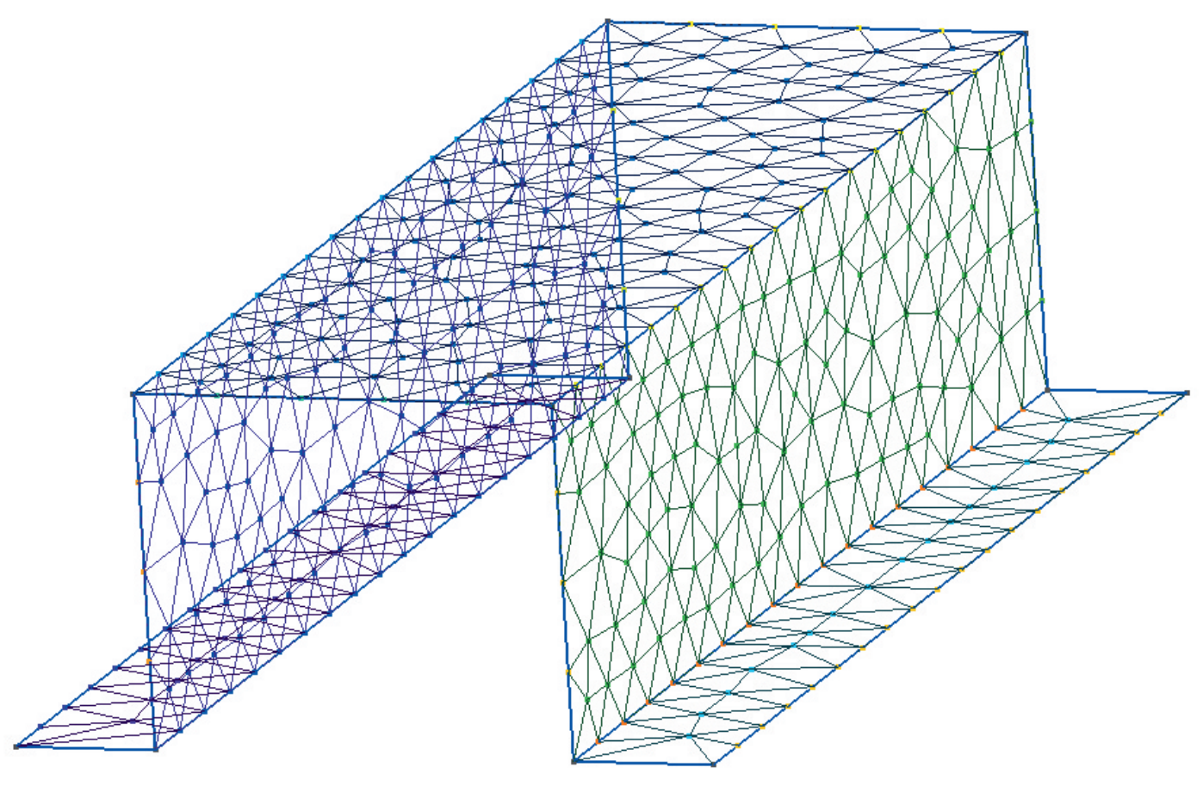
- discretise boundary into elements (lines, triangles, quadrilaterals, ...)
- treecode treats elements as pseudo-particles
- usually, $\bar{\Phi}$ and $\bar{q}$ only known on parts of $\partial\Omega$
- construct system of equations by collocation
- solve iteratively, treecode accelerates matrix-vector product

Supported boundary conditions:

- (mixed) Dirichlet and Neumann
- periodic
- metal wall with floating potential

Complex wall structures

- treecode and BEM allow electrostatic modeling of interaction between plasma and complex wall structures, e.g., castellated tiles
- real world geometries can be modeled in a CAD program like Gmsh



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[3] M. Winkel et al.: A massively parallel, multi-disciplinary Barnes-Hut tree code for extreme-scale *N*-body simulations, Computer Physics Communications **183**, 880-889
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PEPC is freely available at

http://fz-juelich.de/ias/jsc/pepc