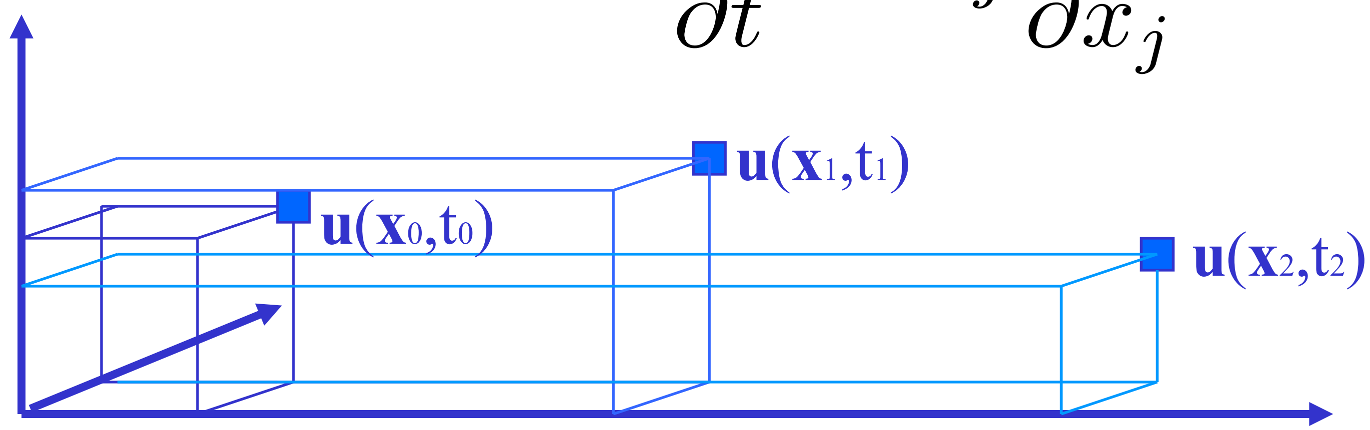
		Course schedule	Required learning
04/07	Class 1	Discretizing differential equations	Discretize differential equations using forward, backward, and central difference, with high order, and evaluate the discretization error
04/11	Class 2	Finite difference methods	Understand stability of low and high order time integration, and use it to solve convection, diffusion, and wave equations
04/14	Class 3	Finite element methods	Understand the concepts of Galerkin methods, test functions, isoparametric elements, and use it to solve elasticity equations.
04/18	Class 4	Spectral methods	Explain the advantages of orthogonal basis functions such as Fourier, Chebyshev, Legendre, and Bessel.
04/21	Class 5	Boundary element methods	Understand the relation between inverse matrices, δ functions and Green's functions, and solve boundary integral equations.
04/25	Class 6	Molecular dynamics	Understand the significance of symplectic time integrators and thermostats, and solve the dynamics of interacting molecules.
04/28	Class 7	Smooth particle hydrodynamics (SPH)	Evaluate the conservation and dissipation properties of differential operators formed from radial basis functions.
05/02	Class 8	Particle mesh methods	How to conserve higher order moments for interpolations schemes when both particle and mesh-based discretizations are used.

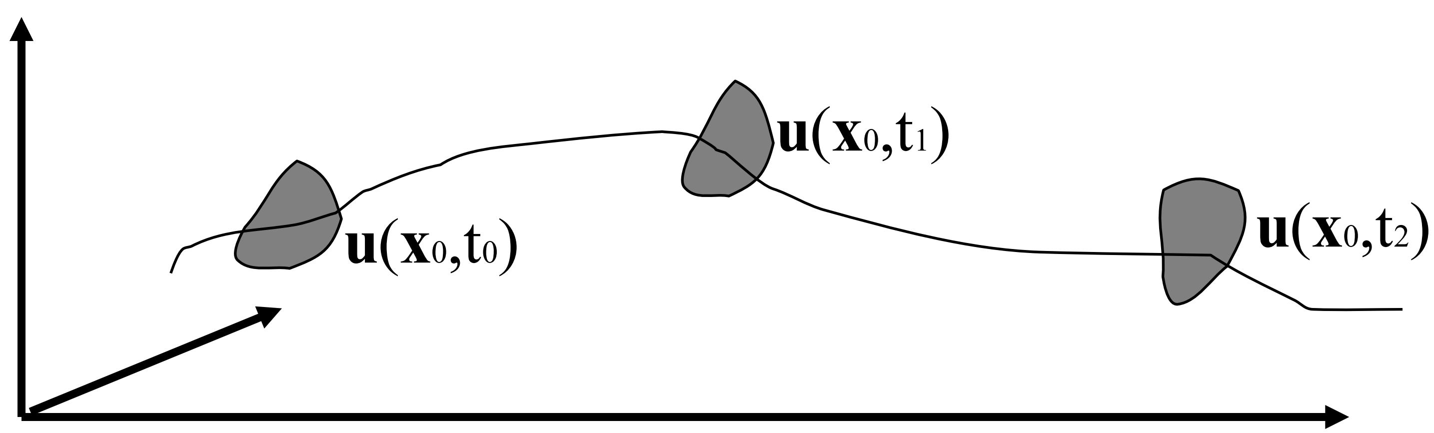
Mesh vs Particle

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho_i}\nabla p_i + \nu \nabla^2 u_i$$



Eulerian

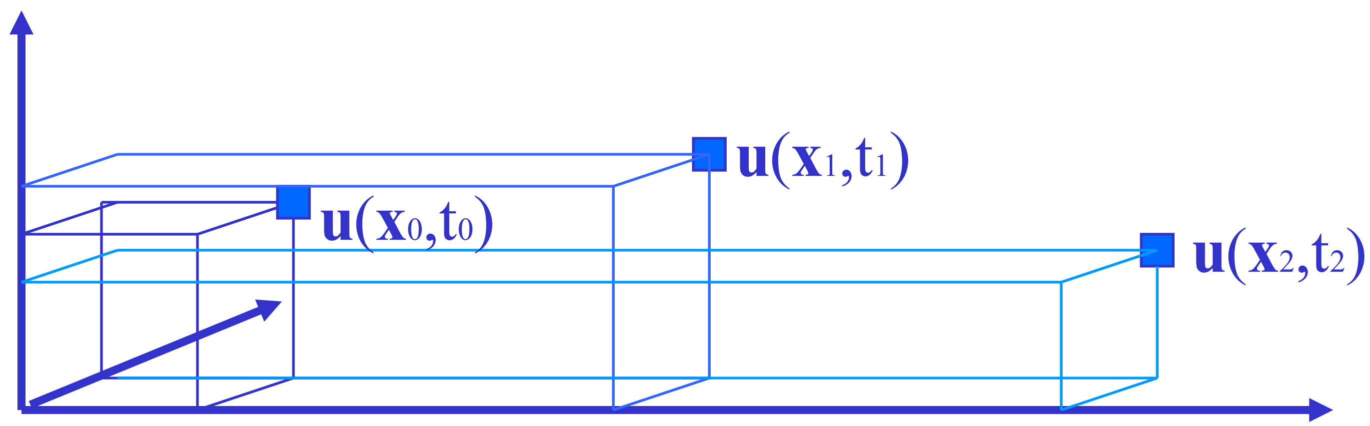
Lagrangian

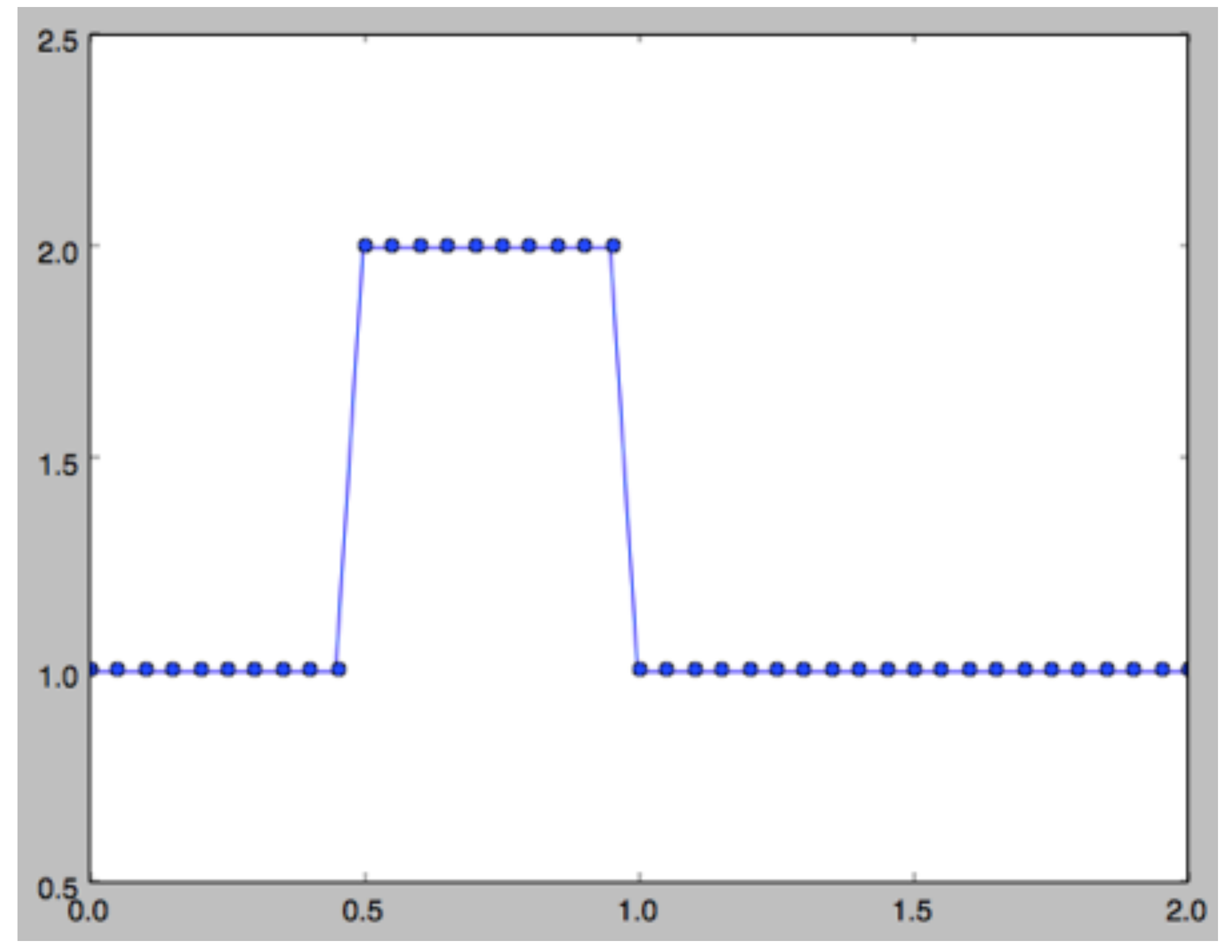


$$\frac{Du_i}{Dt} = -\frac{1}{\rho_i}\nabla p_i + \nu \nabla^2 u_i$$

Finite difference example (step01)

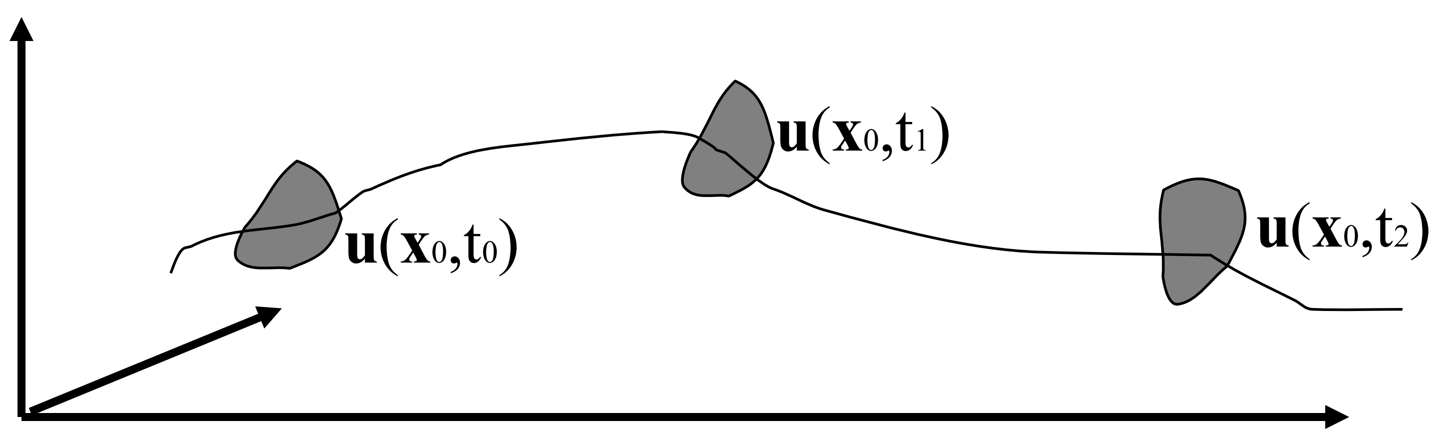
$$\frac{\partial u_i}{\partial t} + c\frac{\partial u_i}{\partial x_j} = 0$$





Eulerian

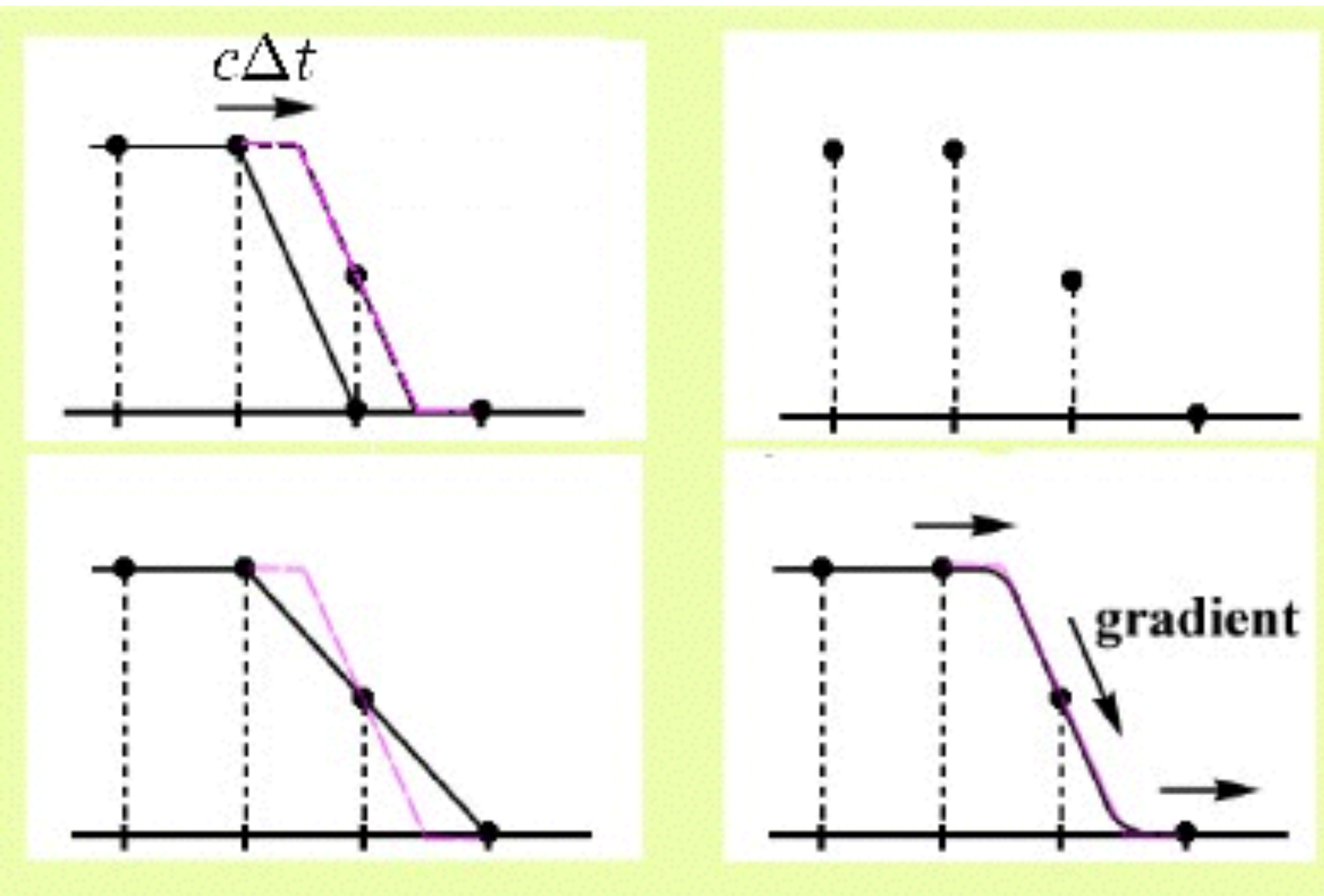
Lagrangian

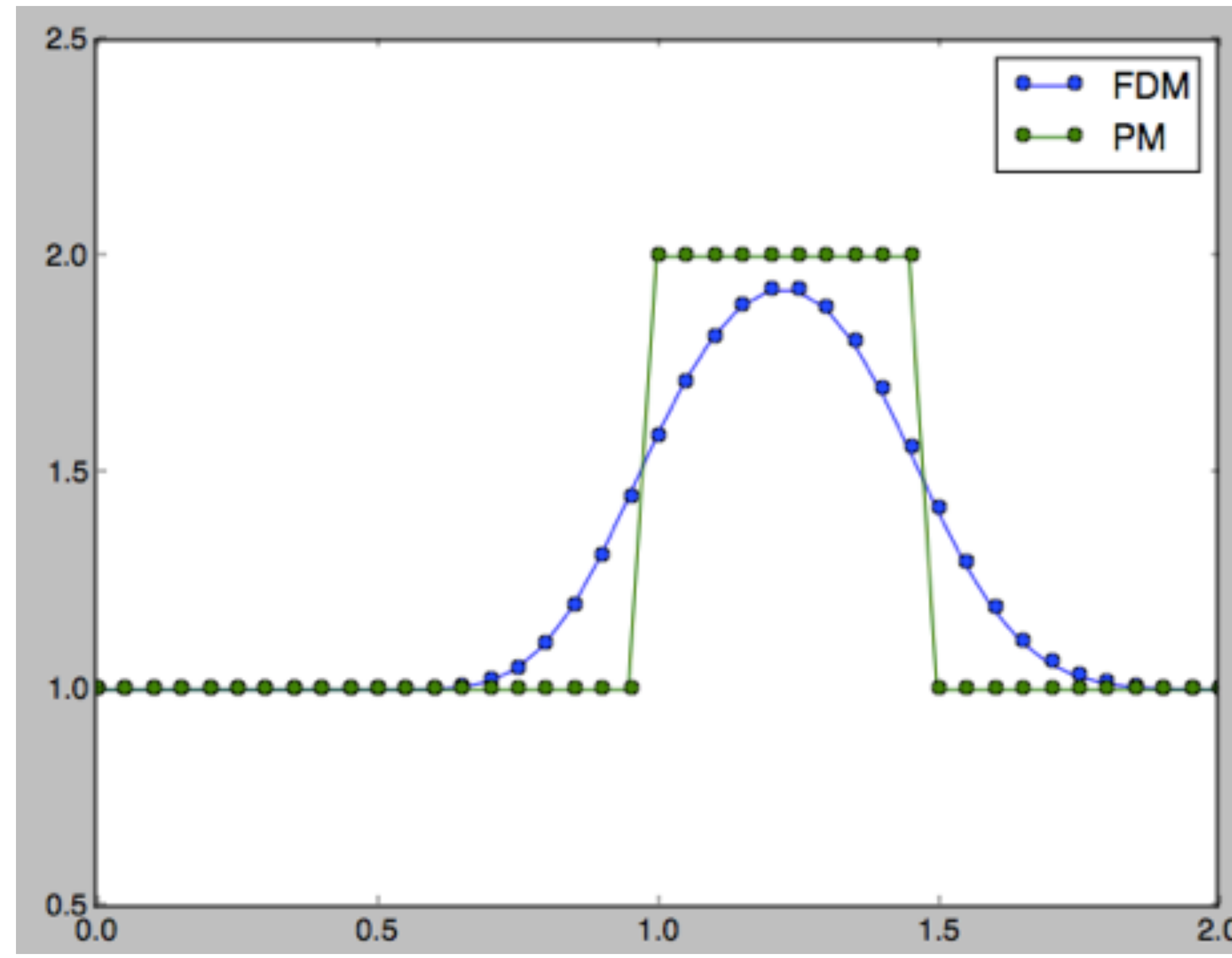


$$\frac{Du_i}{Dt} = 0 \qquad \frac{Dx_i}{Dt} = c$$

No numerical diffusion

$$\frac{\partial u_i}{\partial t} + c\frac{\partial u_i}{\partial x_j} = 0$$

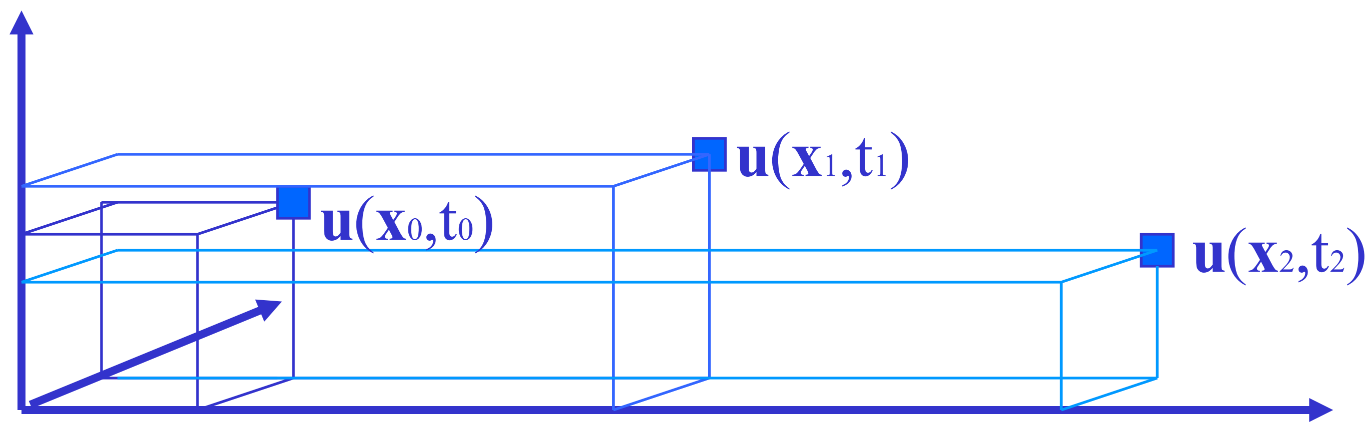


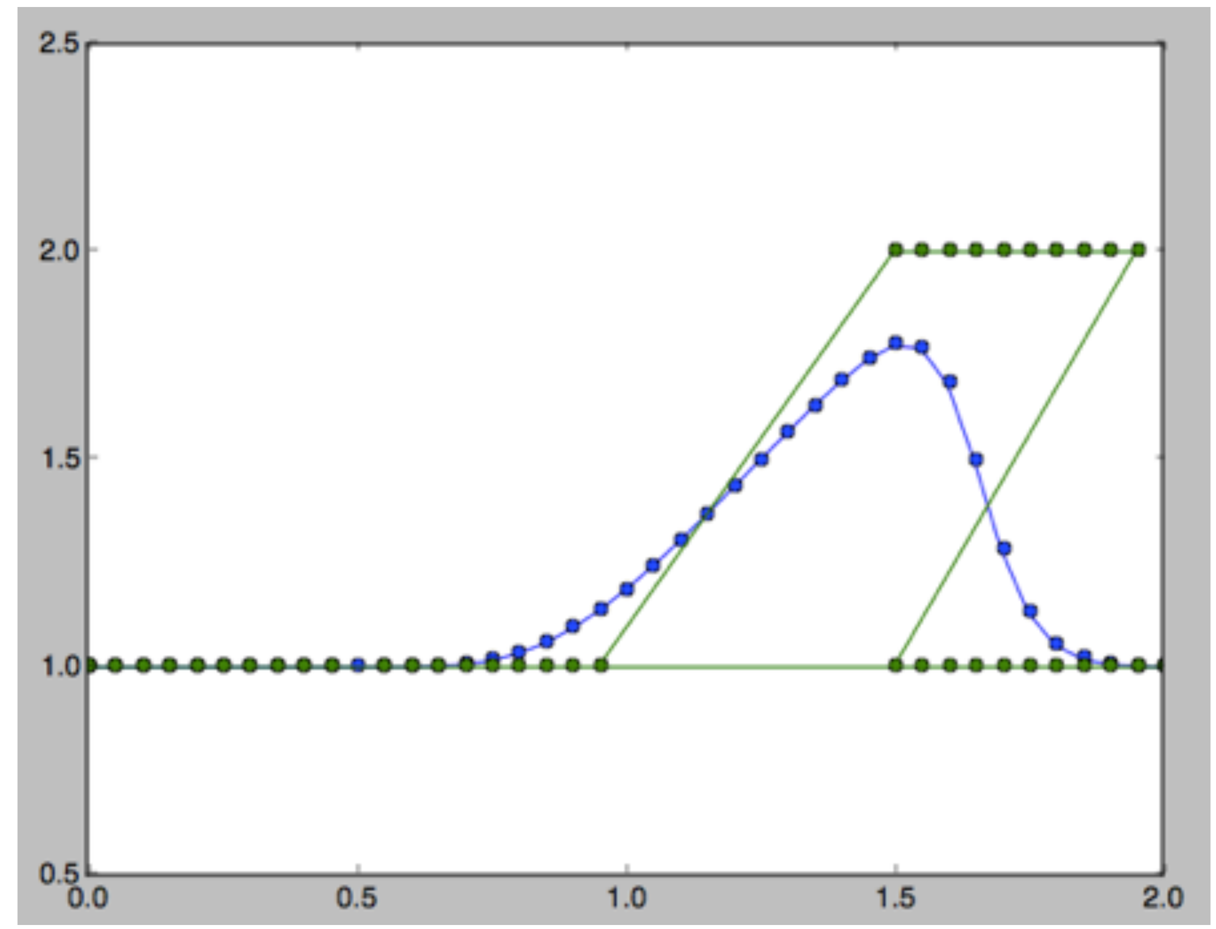


$$\frac{Du_i}{Dt} = 0 \qquad \frac{Dx_i}{Dt} = c$$

Finite difference example (step02)

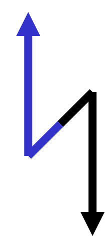
$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = 0$$

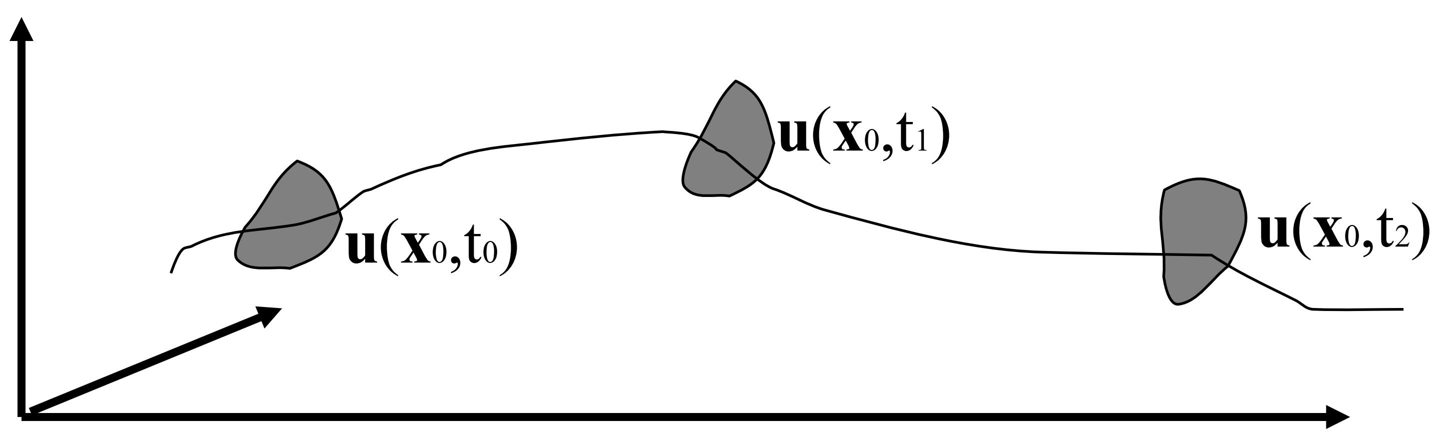




Eulerian

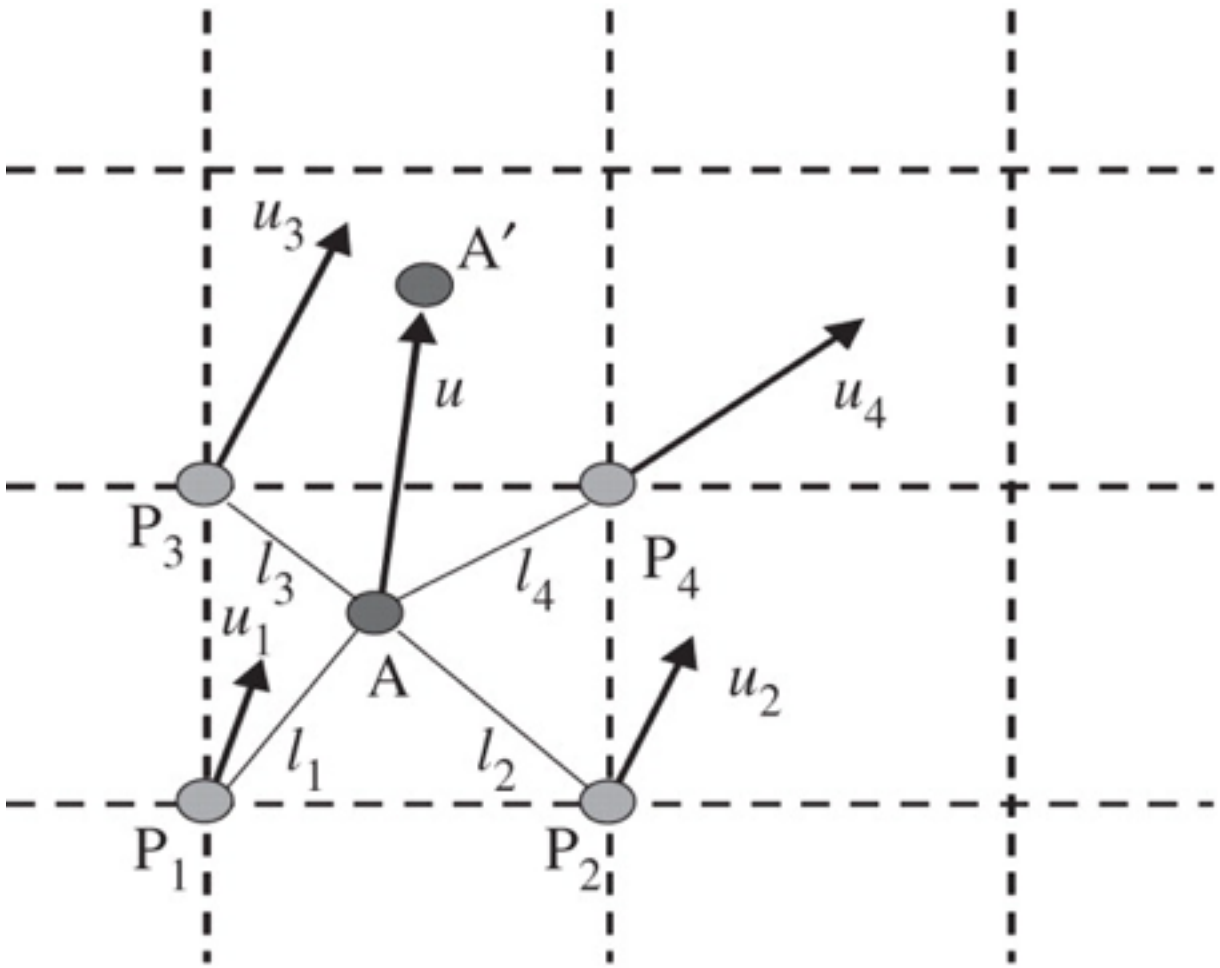
Lagrangian

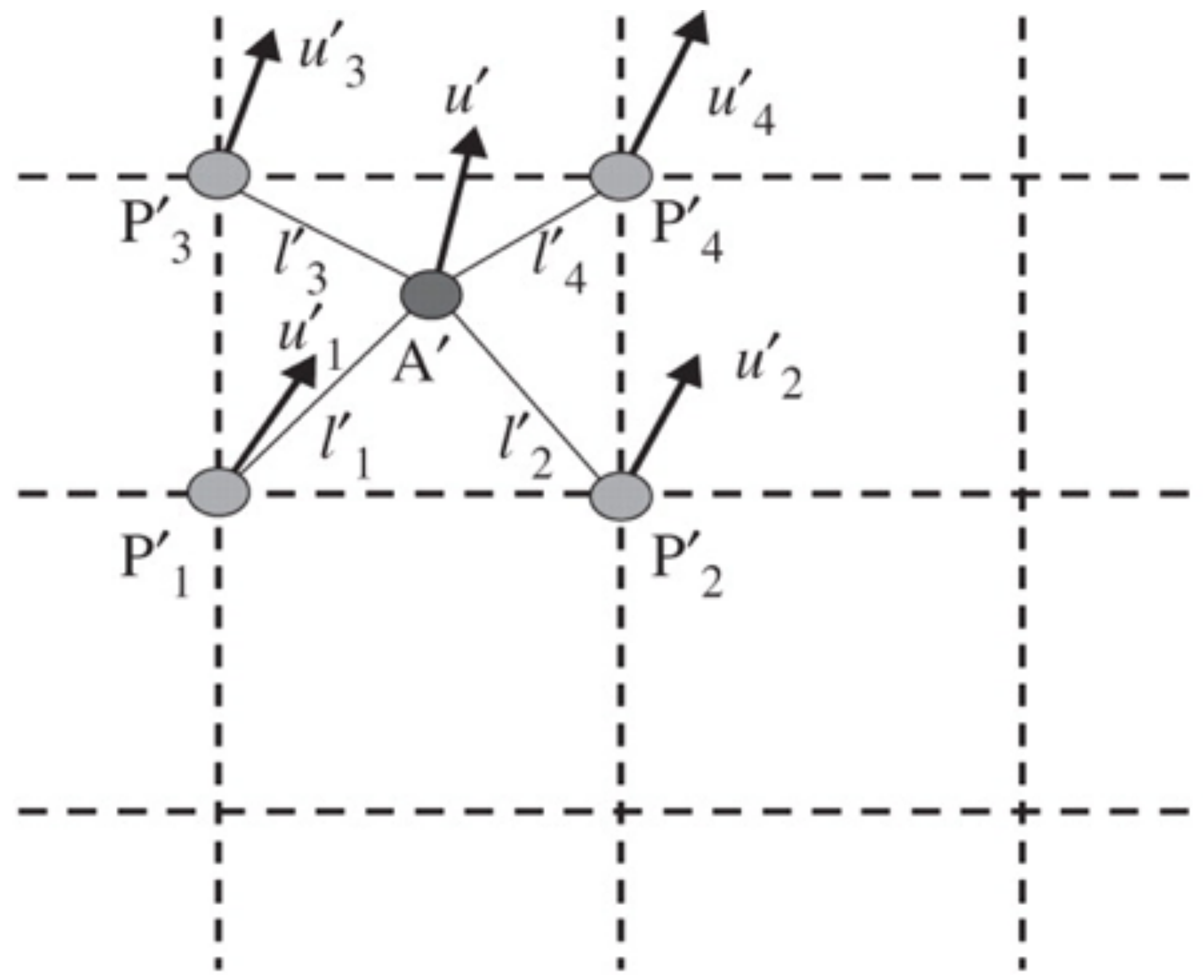




$$\frac{Du_i}{Dt} = 0 \qquad \frac{Dx_i}{Dt} = u_i$$

Interpolate back-and-forth





$$u = \frac{\frac{u_1}{l_1} + \frac{u_2}{l_2} + \frac{u_3}{l_3} + \frac{u_4}{l_4}}{\frac{1}{l_1} + \frac{1}{l_2} + \frac{1}{l_3} + \frac{1}{l_4}}$$

$$u' = \frac{\frac{u'_1}{l'_1} + \frac{u'_2}{l'_2} + \frac{u'_3}{l'_3} + \frac{u'_4}{l'_4}}{\frac{1}{l'_1} + \frac{1}{l'_2} + \frac{1}{l'_3} + \frac{1}{l'_4}}$$

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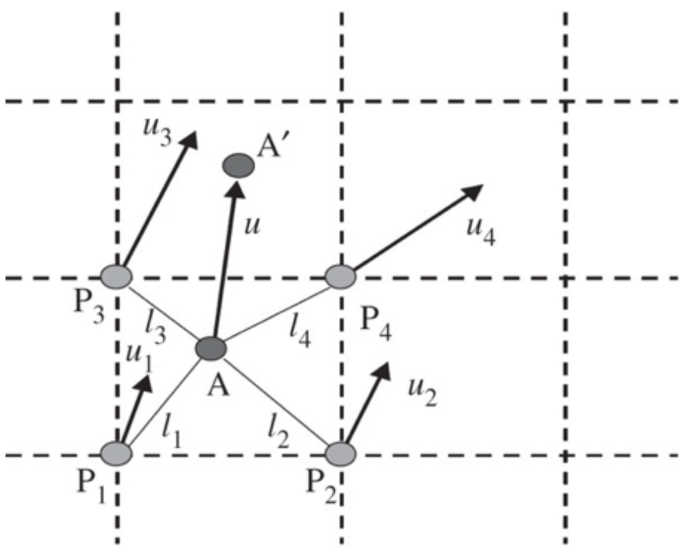
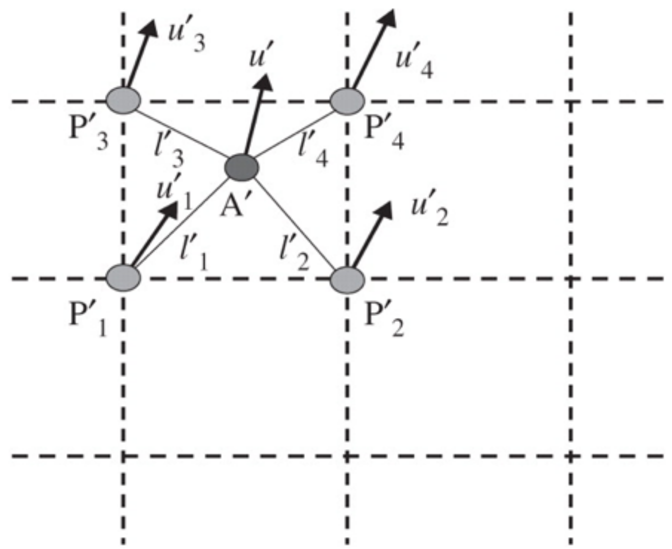
Particle-mesh interpolation (step03)

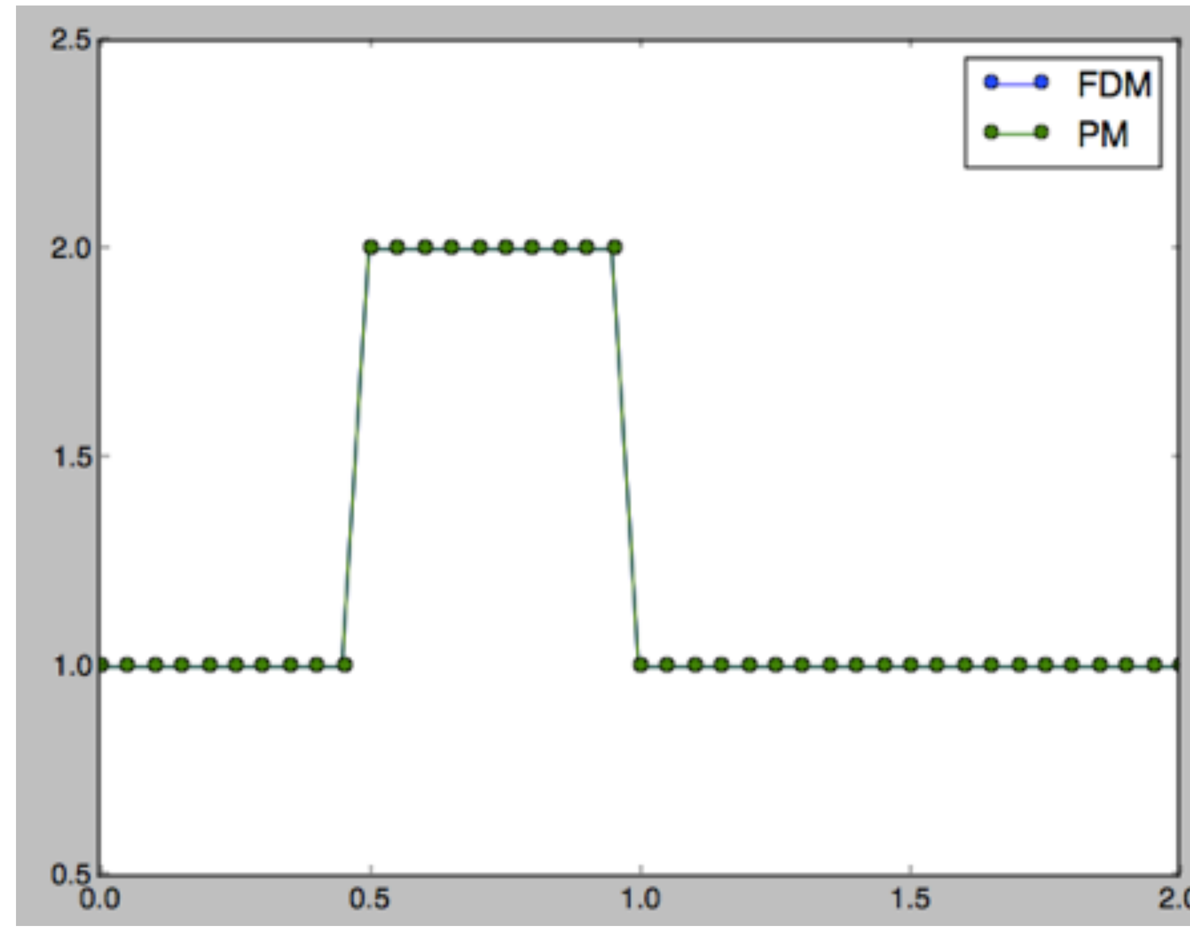
$$\frac{\partial u_i}{\partial t} + c\frac{\partial u_i}{\partial x_j} = 0$$



$$u = \frac{\frac{u_1}{l_1} + \frac{u_2}{l_2} + \frac{u_3}{l_3} + \frac{u_4}{l_4}}{\frac{1}{l_1} + \frac{1}{l_2} + \frac{1}{l_3} + \frac{1}{l_4}}$$



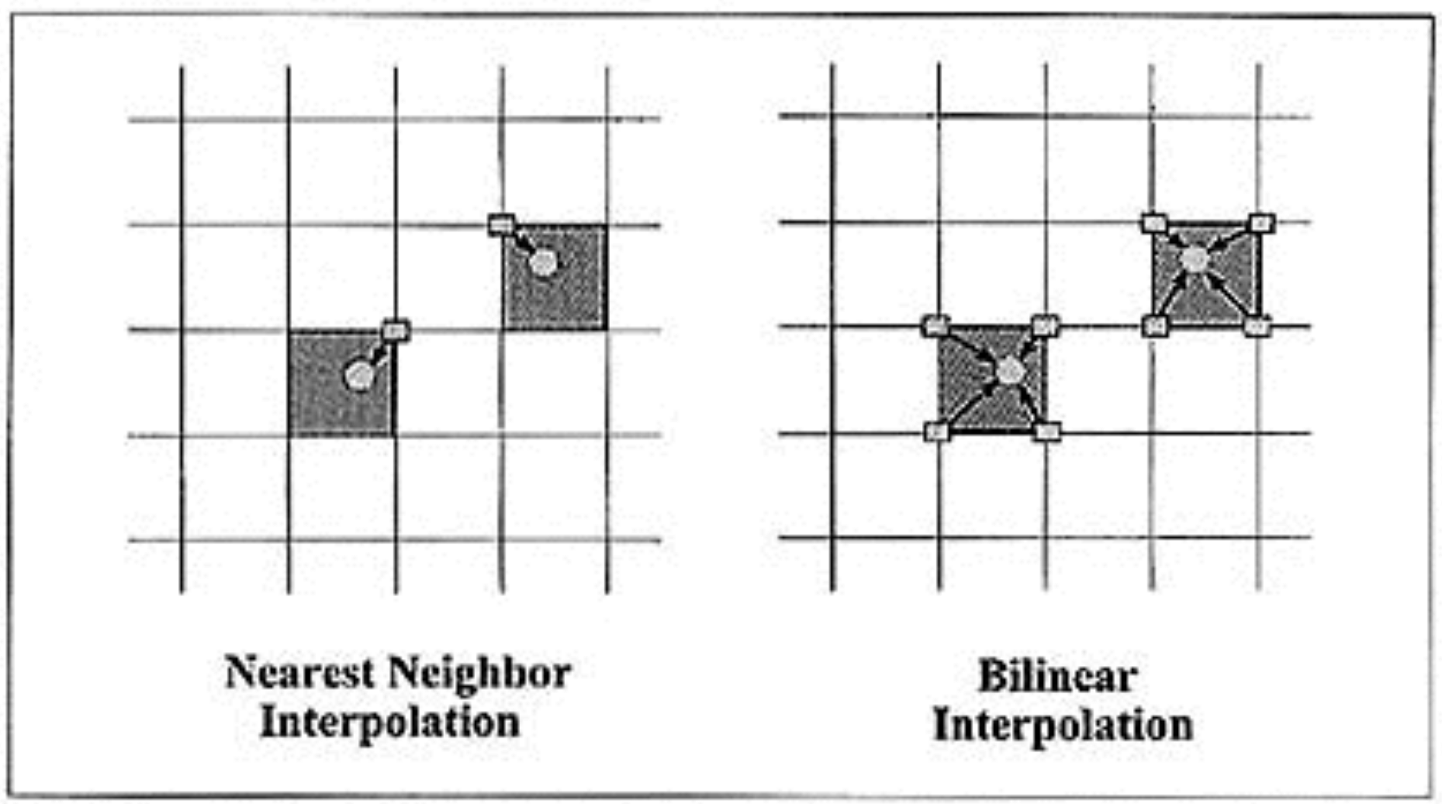
$$u' = \frac{\frac{u'_1}{l'_1} + \frac{u'_2}{l'_2} + \frac{u'_3}{l'_3} + \frac{u'_4}{l'_4}}{\frac{1}{l'_1} + \frac{1}{l'_2} + \frac{1}{l'_3} + \frac{1}{l'_4}}$$

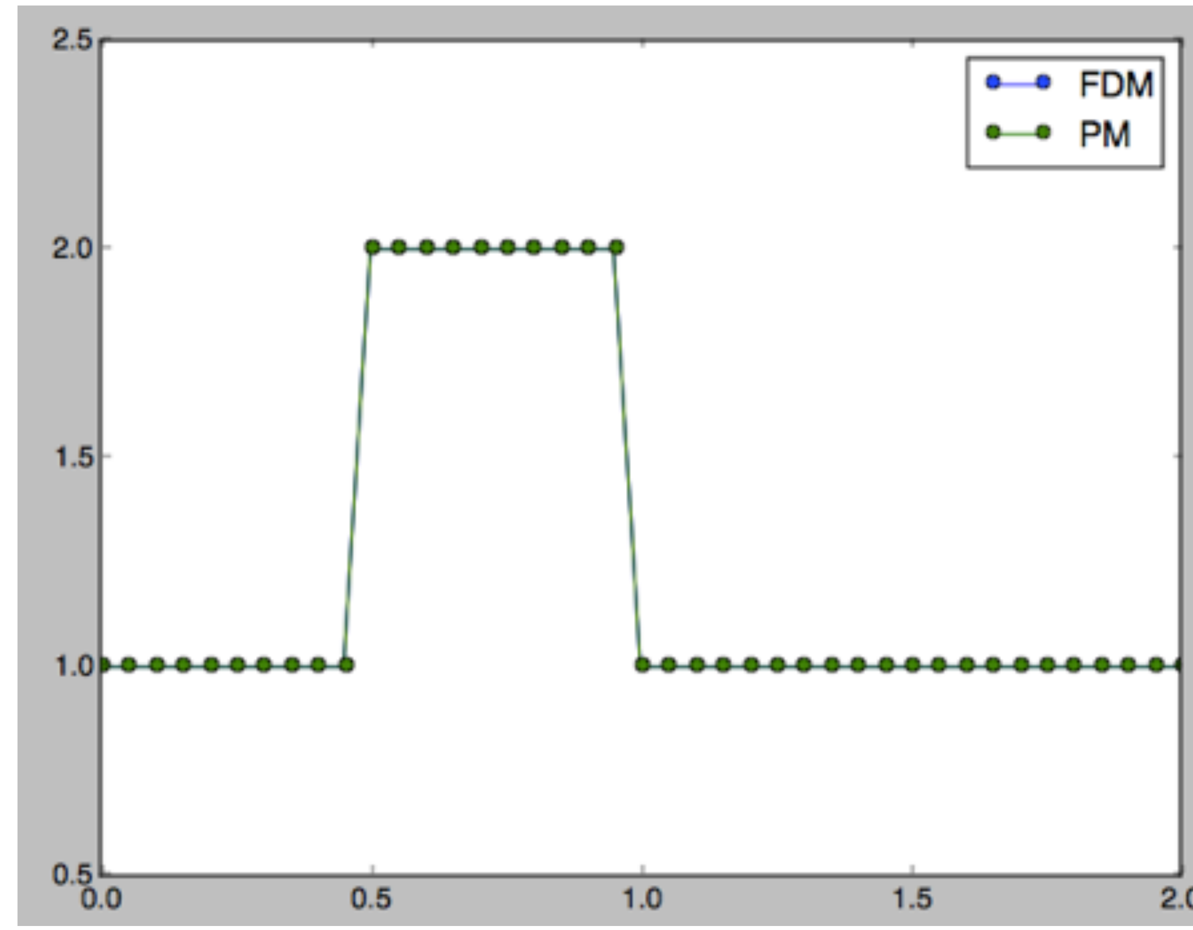


$$\frac{Du_i}{Dt} = 0 \qquad \frac{Dx_i}{Dt} = c$$

Particle-mesh interpolation (step04)

$$\frac{\partial u_i}{\partial t} + c\frac{\partial u_i}{\partial x_j} = 0$$

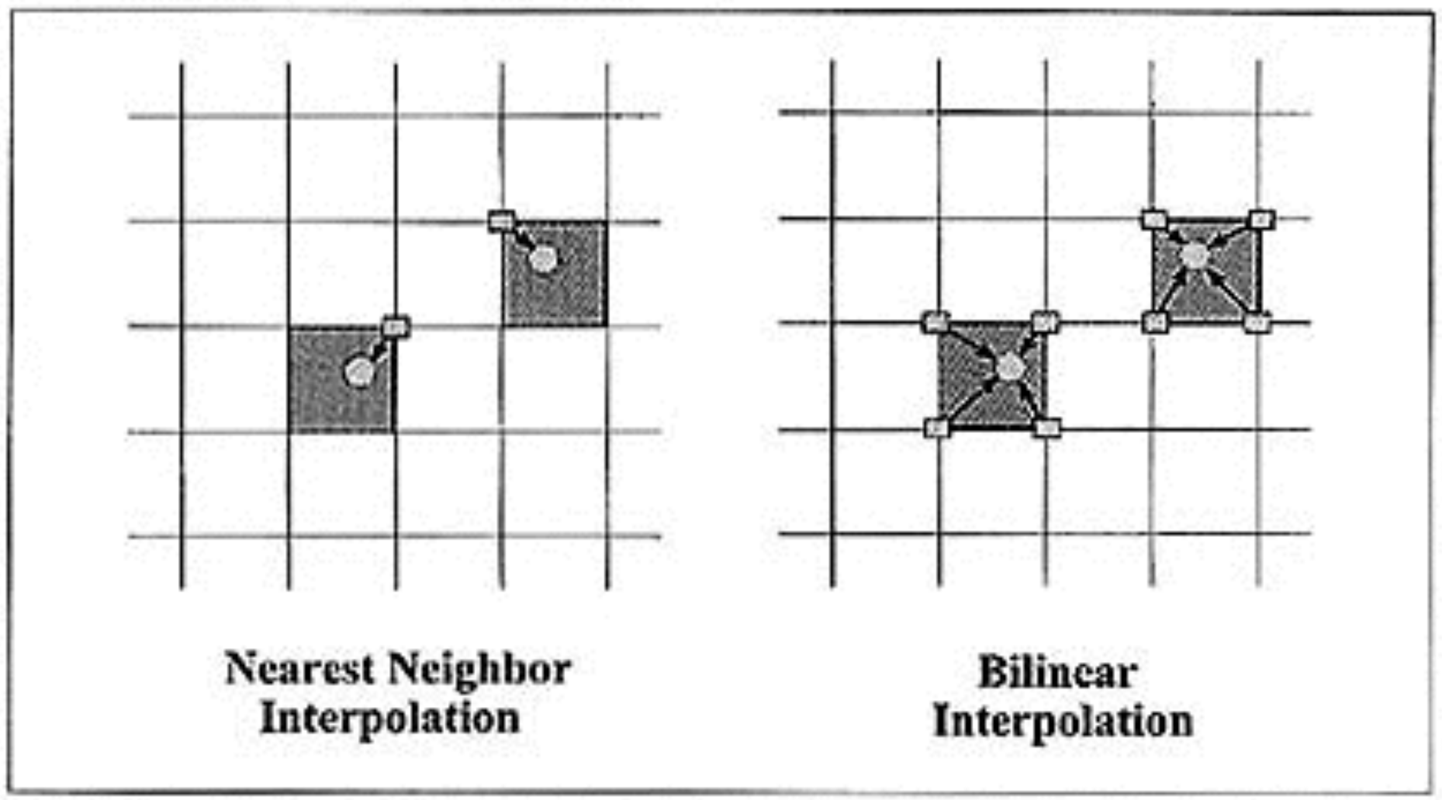


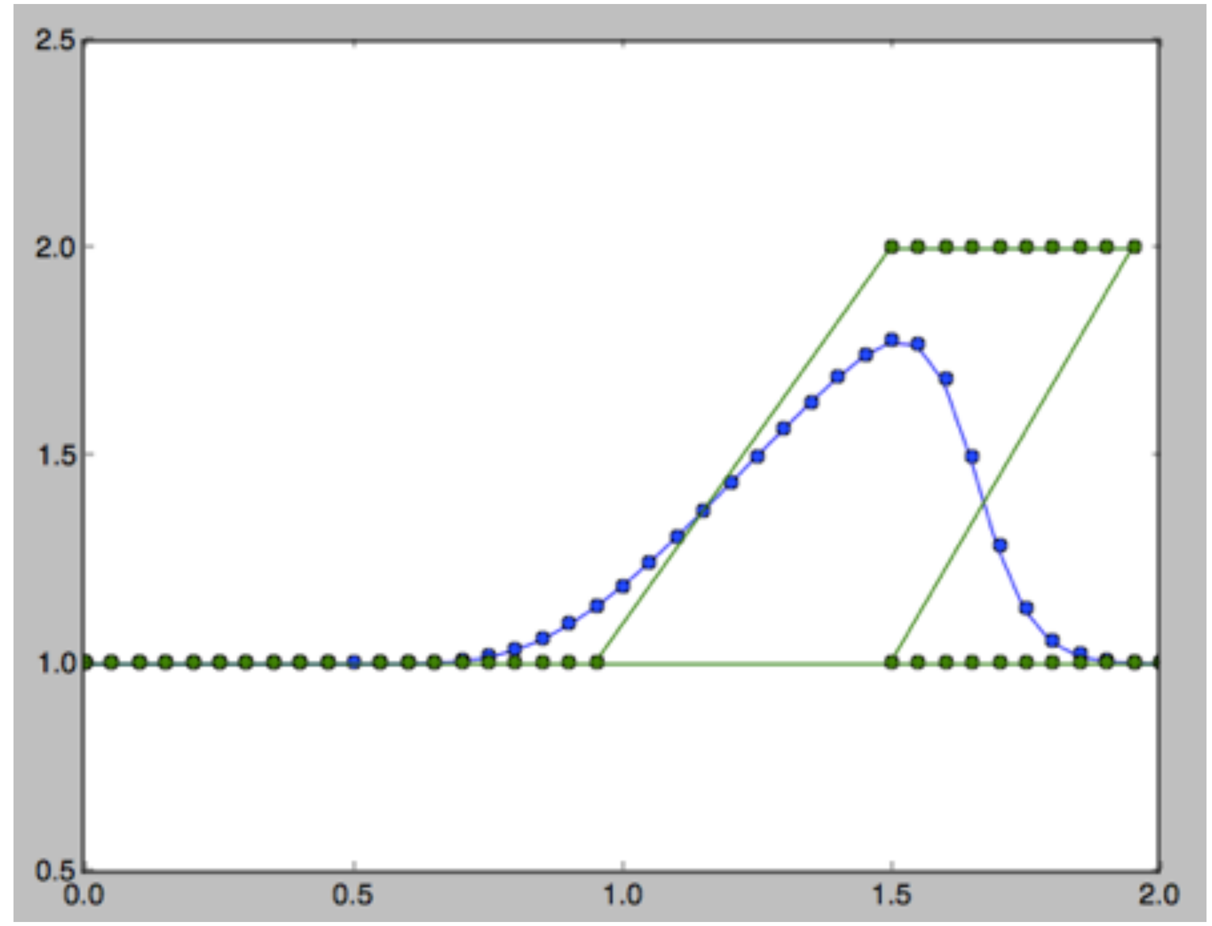


$$\frac{Du_i}{Dt} = 0 \qquad \frac{Dx_i}{Dt} = c$$

Non-linear convection nearest neighbor (step05)

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = 0$$

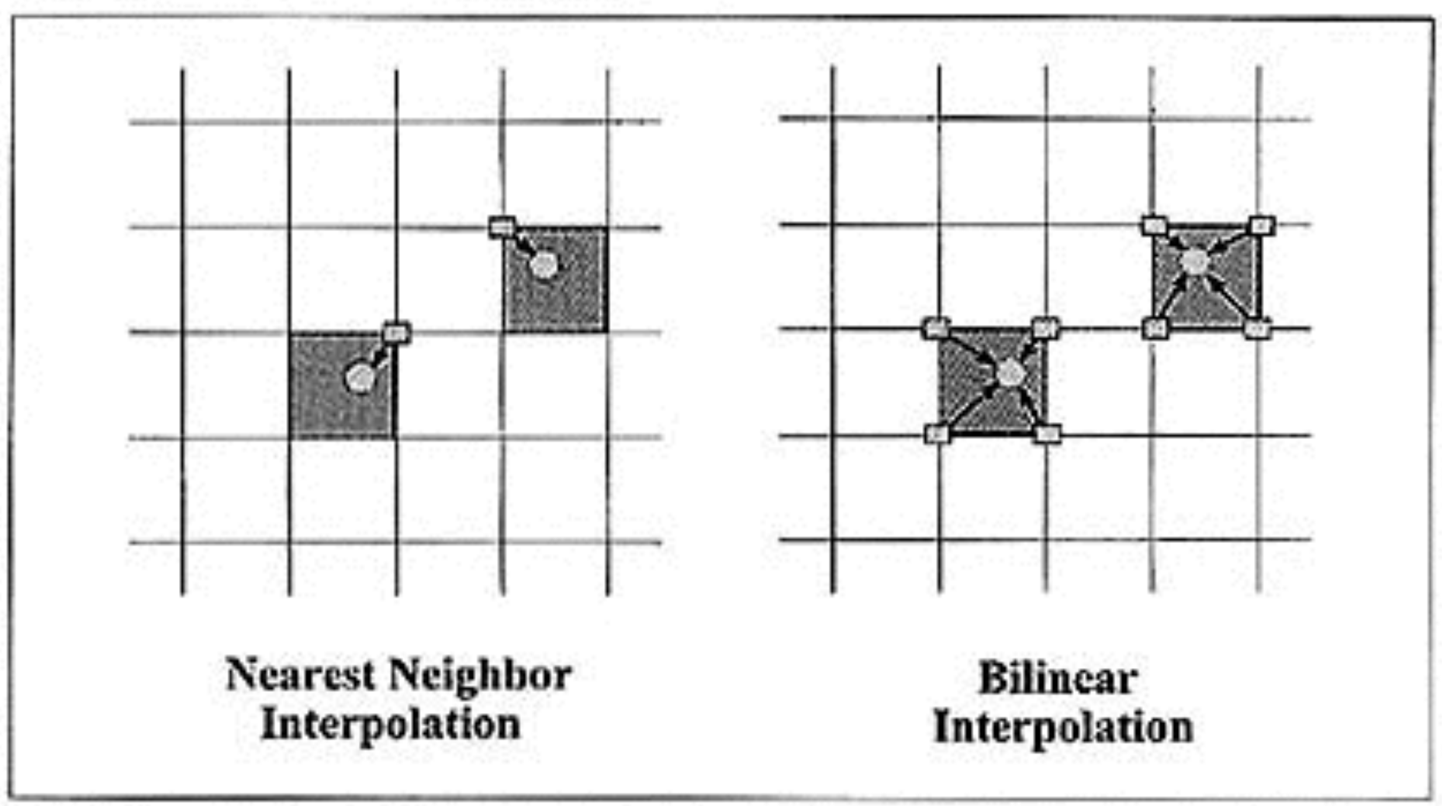


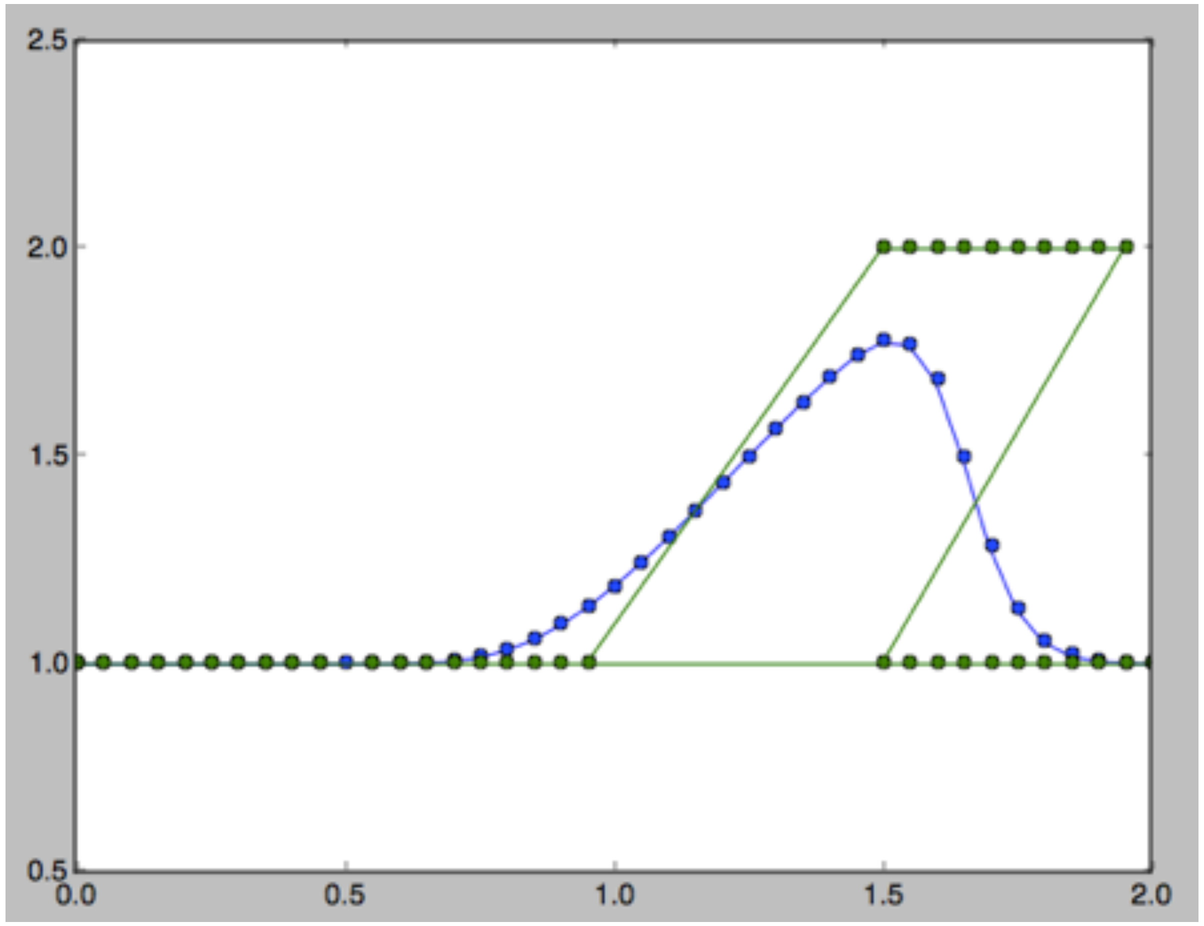


$$\frac{Du_i}{Dt} = 0 \qquad \frac{Dx_i}{Dt} = u_i$$

Non-linear convection interpolation (step06)

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = 0$$





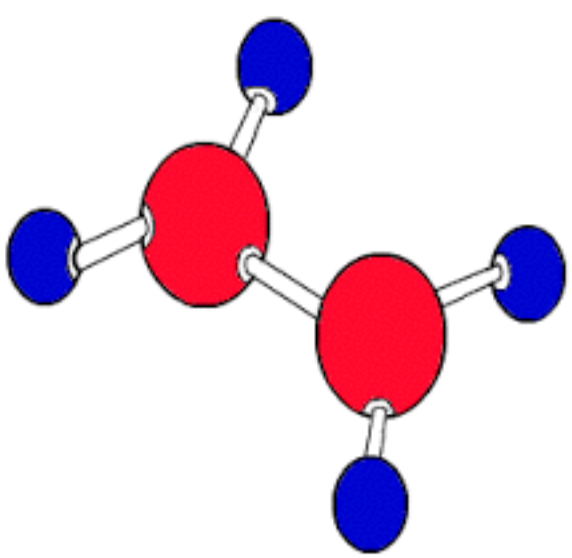
$$\frac{Du_i}{Dt} = 0 \qquad \frac{Dx_i}{Dt} = u_i$$

Particle mesh in molecular dynamics

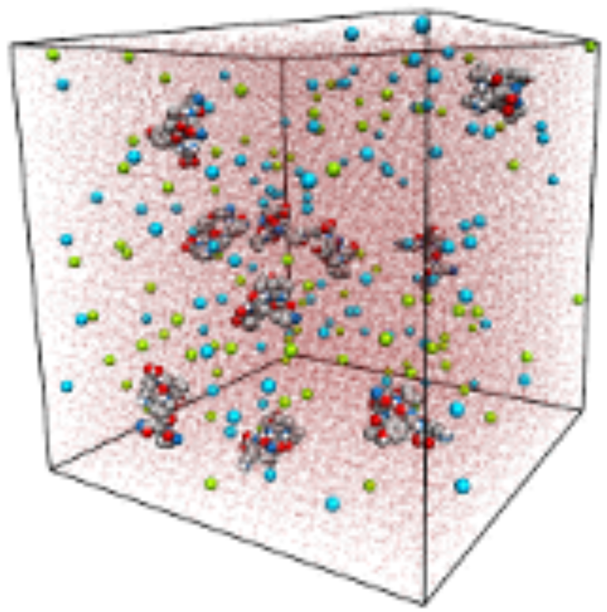
$$U(\vec{R}) = \underbrace{\sum_{bonds} k_i^{bond}(r_i - r_0)^2}_{U_{bond}} + \underbrace{\sum_{angles} k_i^{angle}(\theta_i - \theta_0)^2}_{U_{angle}} +$$

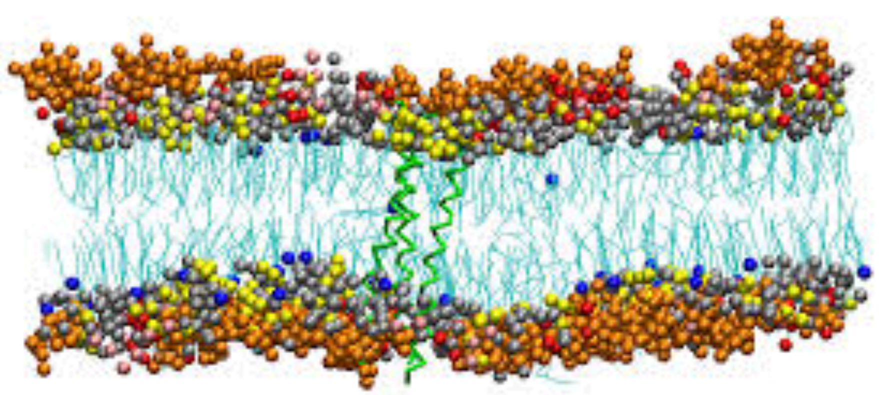
$$\underbrace{\sum_{dihedrals} k_i^{dihe}[1 + \cos(n_i\phi_i + \delta_i)]}_{U_{dihedral}} +$$

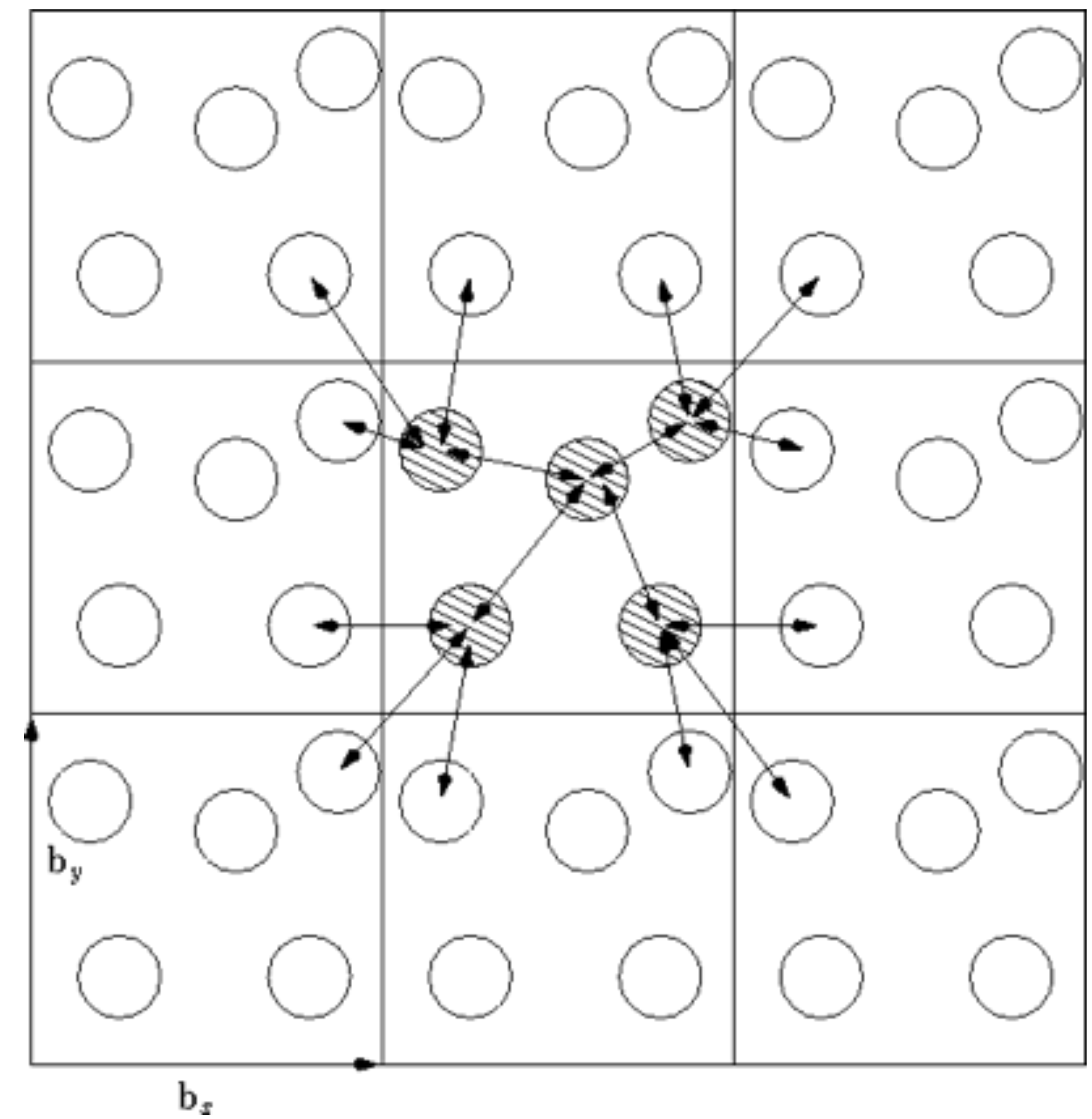
$$\underbrace{\sum_i \sum_{j \neq i} 4\epsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right] + \sum_i \sum_{j \neq i} \frac{q_i q_j}{\epsilon r_{ij}}}_{U_{nonbond}}$$



Periodic boundary conditions

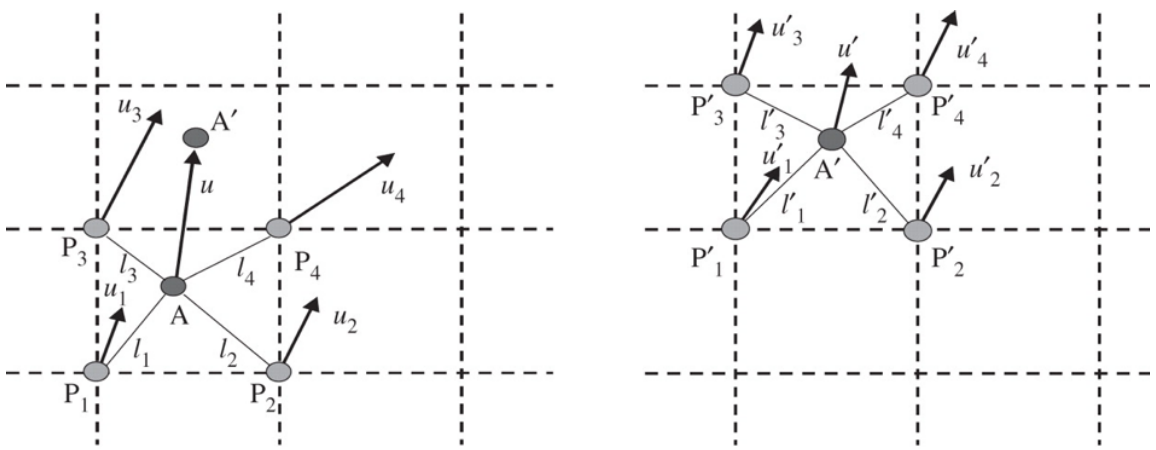






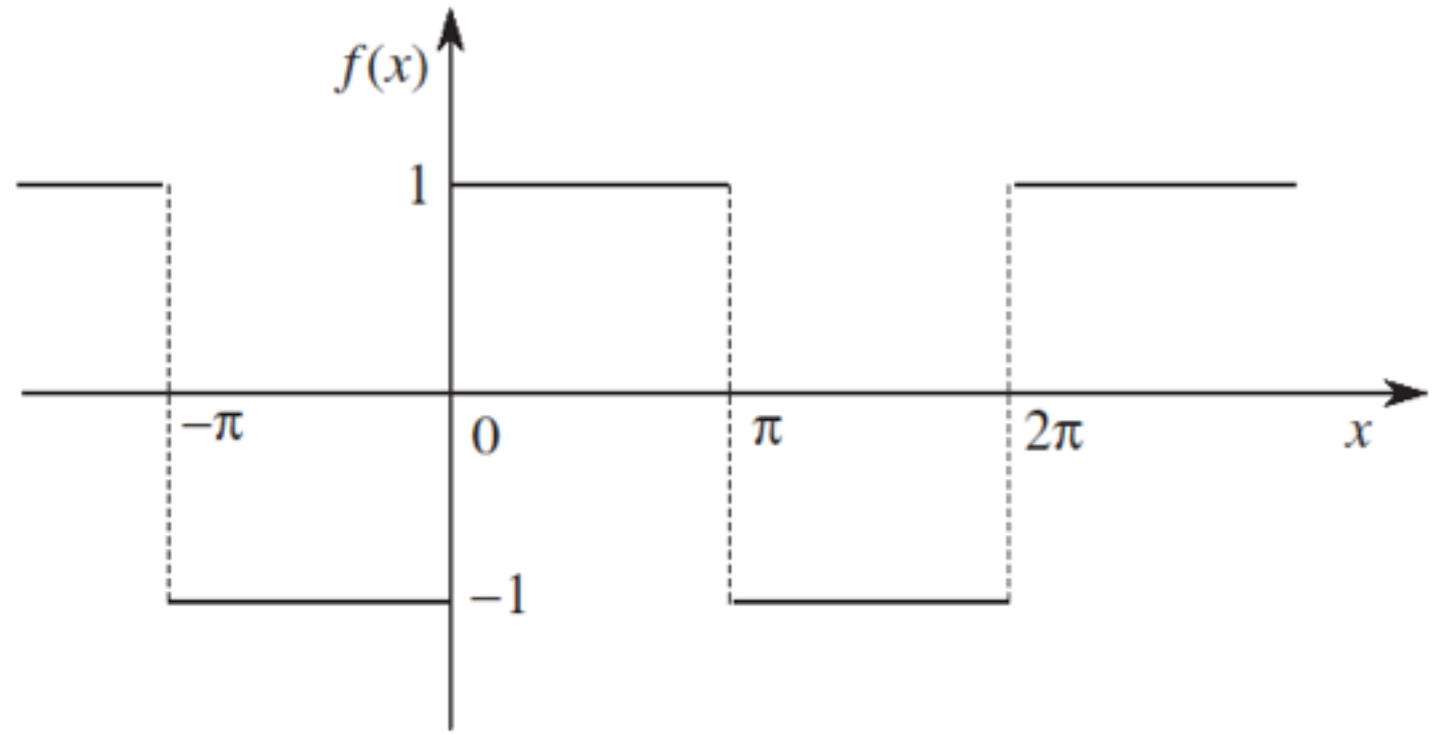
Particle-mesh Ewald

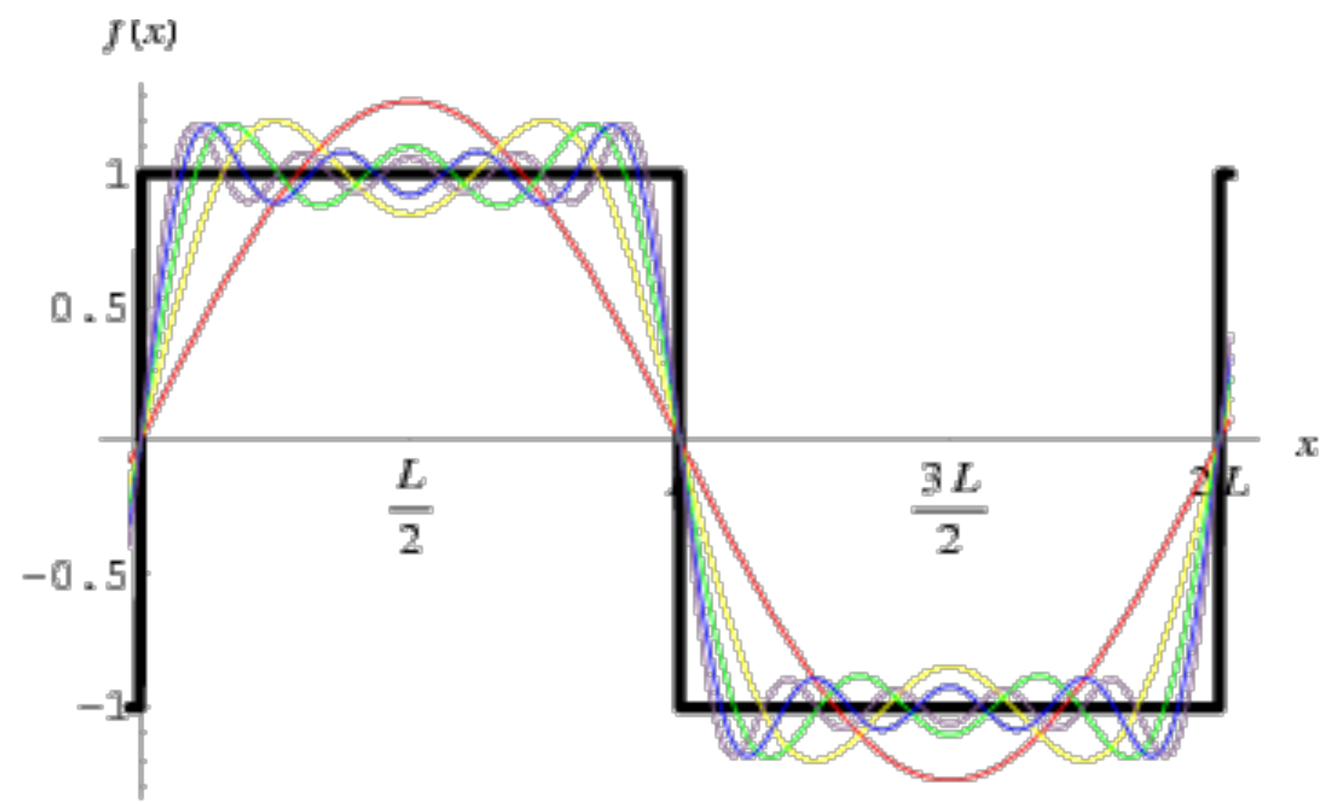
Interpolate onto mesh ⟶ Use FFT to solve in wave space



$$u = \frac{\frac{u_1}{l_1} + \frac{u_2}{l_2} + \frac{u_3}{l_3} + \frac{u_4}{l_4}}{\frac{1}{l_1} + \frac{1}{l_2} + \frac{1}{l_3} + \frac{1}{l_4}}$$

$$u' = \frac{\frac{u'_1}{l'_1} + \frac{u'_2}{l'_2} + \frac{u'_3}{l'_3} + \frac{u'_4}{l'_4}}{\frac{1}{l'_1} + \frac{1}{l'_2} + \frac{1}{l'_3} + \frac{1}{l'_4}}$$





05/09	Class 9	Dense direct solvers	Understand the principle of LU decomposition and the optimization and parallelization techniques that lead to the LINPACK benchmark.
05/12	Class 10	Dense eigensolvers	Determine eigenvalues and eigenvectors and understand the fast algorithms for diagonalization and orthonormalization.
05/16	Class 11	Sparse direct solvers	Understand reordering in AMD and nested dissection, and fast algorithms such as skyline and multifrontal methods.
05/19	Class 12	Sparse iterative solvers	Understand the notion of positive definiteness, condition number, and the difference between Jacobi, CG, and GMRES.
05/23	Class 13	Preconditioners	Understand how preconditioning affects the condition number and spectral radius, and how that affects the CG method.
05/26	Class 14	Multigrid methods	Understand the role of smoothers, restriction, and prolongation in the V-cycle.
05/30	Class 15	Fast multipole methods, H-matrices	Understand the concept of multipole expansion and low-rank approximation, and the role of the tree structure.