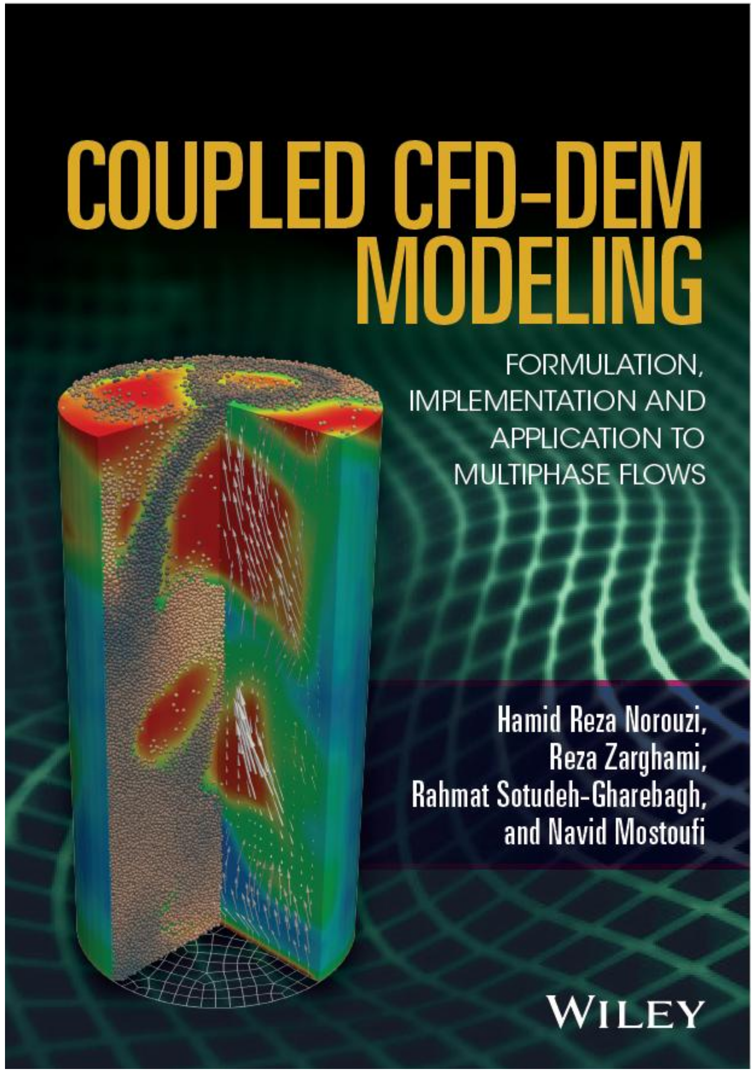
Basics of DEM

Reference


COUPLED CFD-DEM MODELING
FORMULATION, IMPLEMENTATION AND APPLICATION TO MULTIPHASE FLOWS
Hamid Reza Norouzi,
Reza Zarghami,
Rahmat Sotudeh-Gharebagh,
and Navid Mostoufi
WILEY

DEM approaches

- Hard-sphere:
  - No deformation/overlap between particles are allowed
  - Instantaneous and pair-wise contacts
  - Applicable to **dilute systems**

- Soft-sphere:
  - Particles are allowed to have slight overlap
  - Each contact may last for a period of time (processed for multiple time steps)
  - A particle with multiple contacts is possible
  - Applicable to **dilute to dense system**
  - Adding LRF is straight forward

Basic Equations

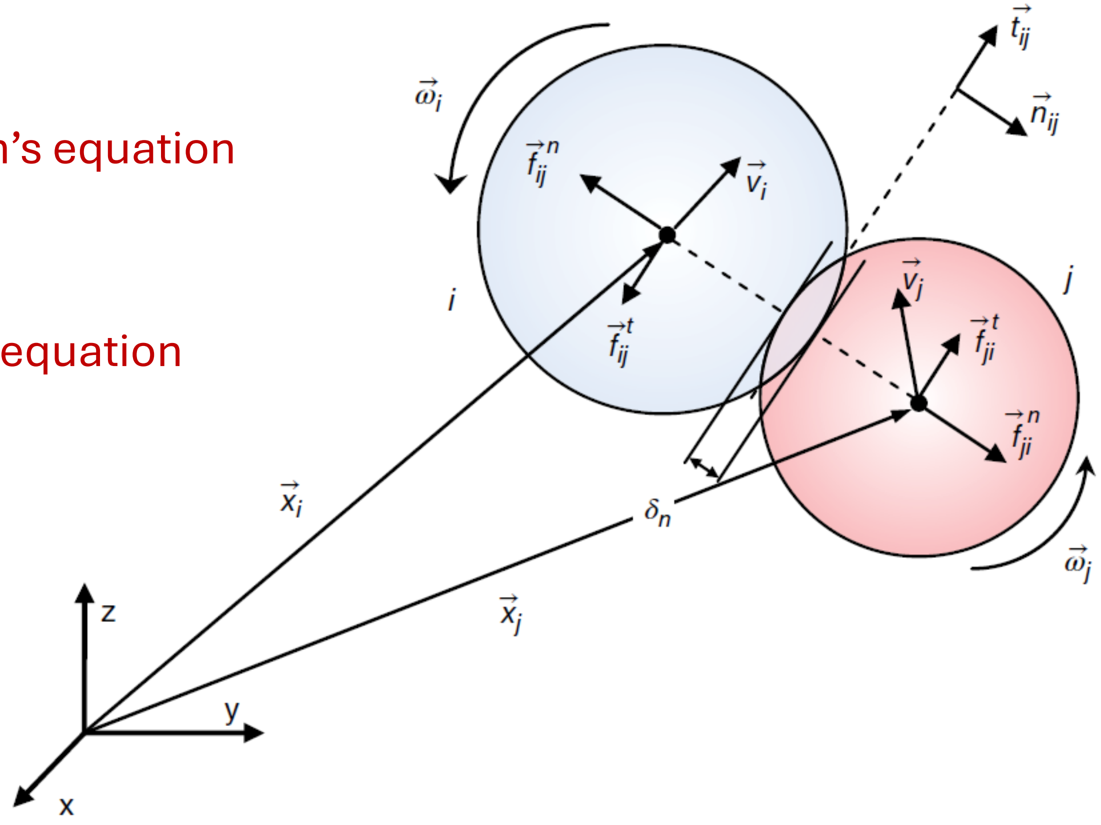
- For each spherical particle *i*:

$$m_i \frac{d\vec{v}_i}{dt} = m_i \frac{d^2\vec{x}_i}{dt^2} = \sum_{j \in CL_i} \vec{f}_{ij}^{\,p-p} + \vec{f}_i^{\,f-p} + m_i\vec{g}$$

Newton's equation

$$I_i \frac{d\vec{\omega}_i}{dt} = \sum_{j \in CL_i} \left(\vec{M}_{ij}^{\,t} + \vec{M}_{ij}^{\,r}\right)$$

Euler's equation

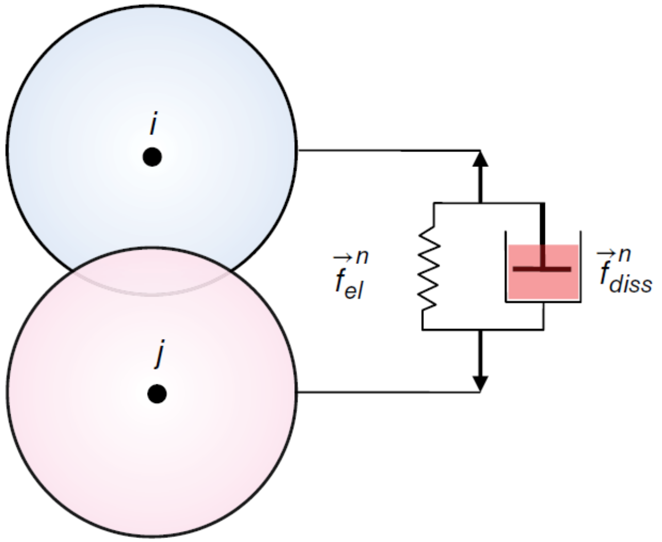


Linear Contact Force

- Normal contact force:

$$\vec{f}_{ij}^{\,n} = \vec{f}_{el}^{\,n} + \vec{f}_{diss}^{\,n} = -\left(k_n \delta_n\right)\vec{n}_{ij} - \left(\eta_n v_{rn}\right)\vec{n}_{ij}$$

$$\eta_n = \frac{-2\ln e_n \sqrt{m_{eff} k_n}}{\sqrt{\left(\ln e_n\right)^2 + \pi^2}}$$



- Tangential contact force:

$$\vec{f}_{ij}^{\,t} = \vec{f}_{el}^{\,t} + \vec{f}_{diss}^{\,t} = -\left(k_t \delta_t\right)\vec{t}_{ij} - \left(\eta_t v_{rt}\right)\vec{t}_{ij}$$

- Friction:

$$\vec{f}_{ij}^{\,t} = -\mu \vec{f}_{ij}^{\,n} \operatorname{sgn}\left(\delta_t\right)\vec{t}_{ij} \qquad \vec{M}_{ij}^{\,r} = -\mu_r R_{eff} \left|\vec{f}_{ij}^{\,n}\right| \hat{\omega}_{ij}$$

Non-linear model

- Normal contact force:

$$\vec{f}_{ij}^{\,n} = \vec{f}_{el}^{\,n} + \vec{f}_{diss}^{\,n} = \left(-\frac{4}{3} \underline{E_{eff}} \sqrt{R_{eff}}\, \delta_n^{3/2} \right) \vec{n}_{ij} - \left(\underline{\tilde{\eta}_n} \delta_n^{1/4} v_{rn} \right) \vec{n}_{ij}$$

$$\tilde{\eta}_n = \frac{-2.2664 \ln e_n \sqrt{m_{eff} \tilde{k}_{Hertz}}}{\sqrt{\left(\ln \underline{e_n} \right)^2 + 10.1354}}$$

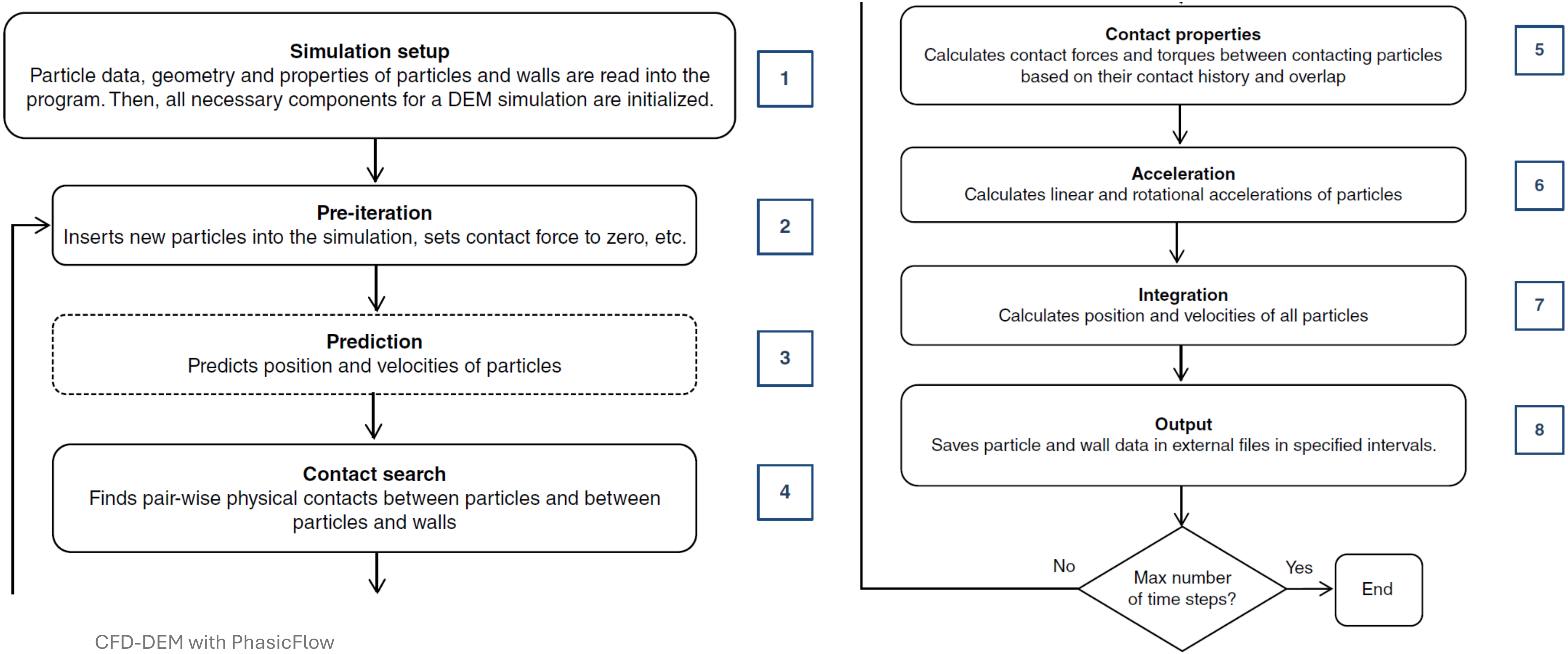
- Tangential contact force:

$$\vec{f}_{ij}^{\,t} = \vec{f}_{el}^{\,t} = -8 \underline{G_{eff}} \sqrt{R_{eff}}\, \delta_n^{1/2} \delta_t \vec{t}_{ij}$$

  - Friction

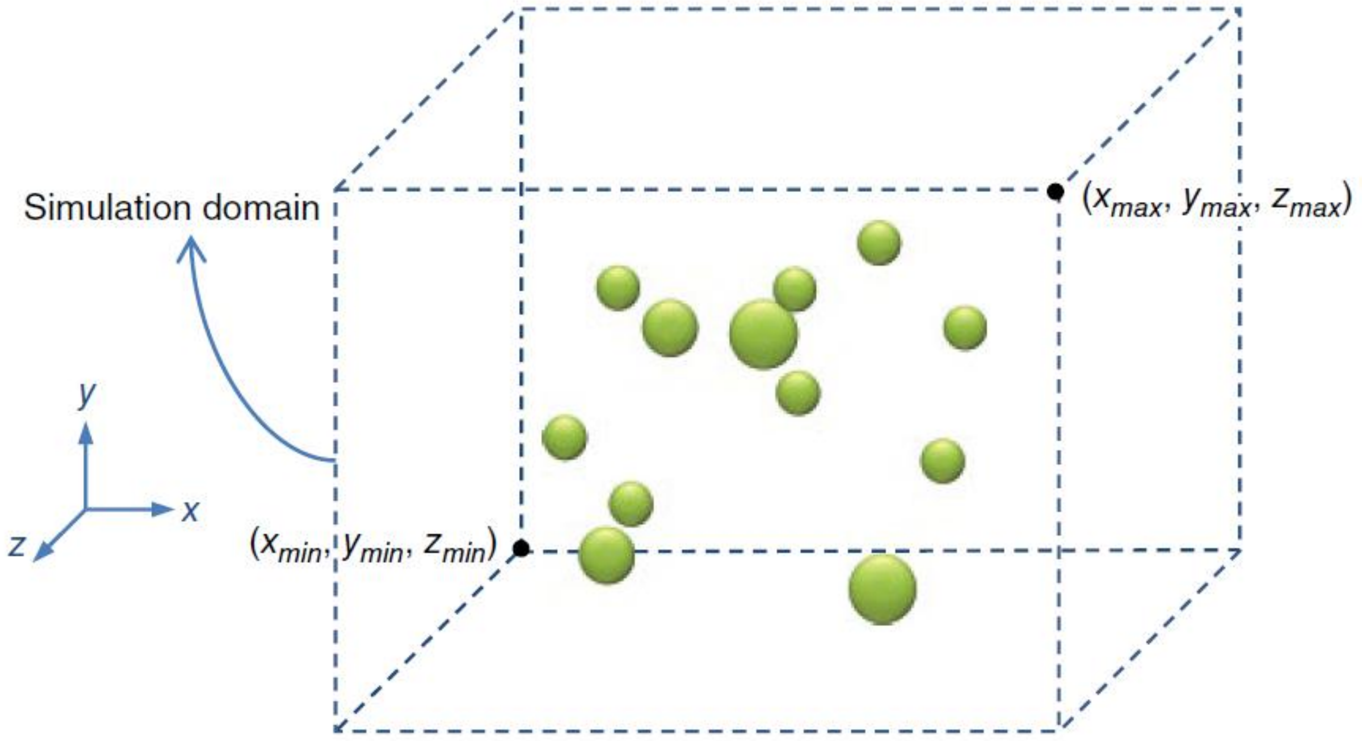
$$\vec{f}_{ij}^{\,t} = -\underline{\mu} \vec{f}_{ij}^{\,n} \operatorname{sgn}(\delta_t) \vec{t}_{ij} \qquad \vec{M}_{ij}^{\,r} = -\underline{\mu_r} R_{eff} \left| \vec{f}_{ij}^{\,n} \right| \hat{\omega}_{ij}$$

DEM calculation steps



Contact Search (1)

- Simulation domain



Contact Search (2)

- No Binary Search (NBS)

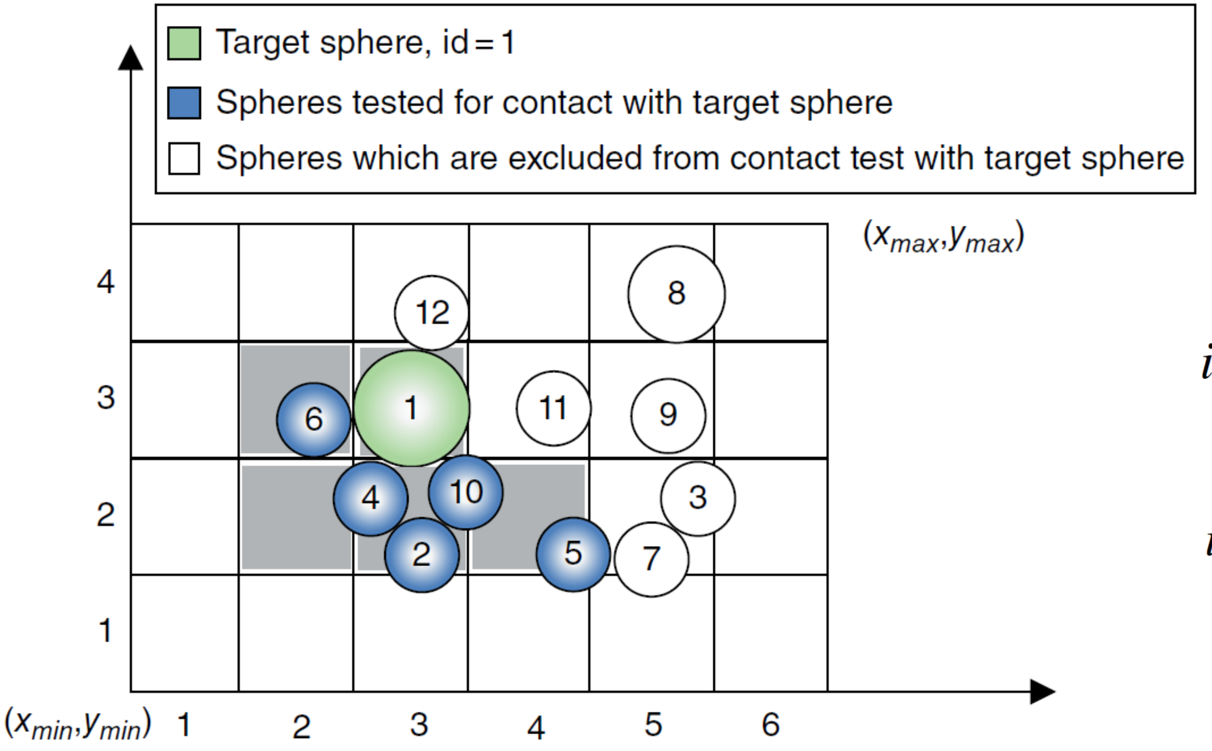


Figure 3.4 Discretized simulation domain and bounding sphere in 2D space

$$ix = \mathrm{int}\left(\frac{x_i - x_{min}}{dx}\right) + 1$$

$$iy = \mathrm{int}\left(\frac{y_i - y_{min}}{dx}\right) + 1$$

Integration of equations (1)

- DEM uses **explicit** integration
  - To avoid instabilities, the time step of integration should be less than period that it takes to transmit a wave from one particle to another

Linear model

$$\Delta t_{crit} \propto 2\pi\sqrt{\frac{m}{k}}$$

Non-Linear model

$$\Delta t_{crit} = \frac{\pi R_p}{\chi}\sqrt{\frac{\rho}{G}} \qquad \chi = 0.1631\nu + 0.8766$$

- This requires integration time step around **1.0×10^{-6}** and **1.0×10^{-5}** s
  - This is achieved by **reduced** values of *k* or *Y*.

Time step should be **a fraction** of this critical time step

Integration of equations (2)

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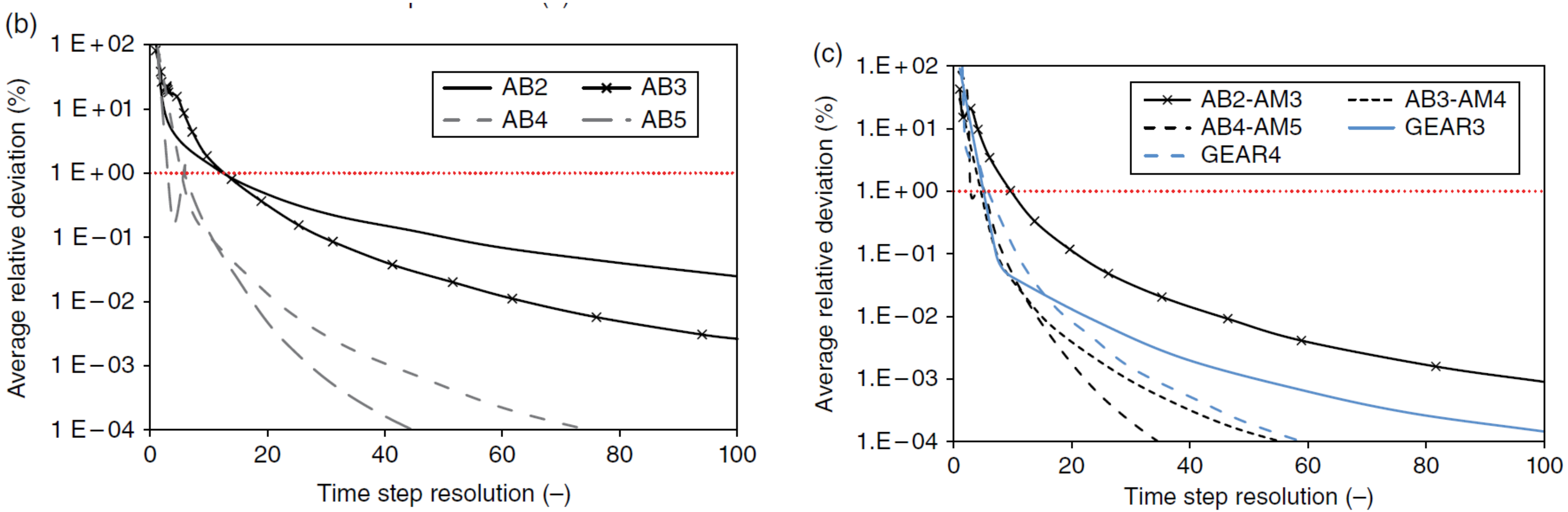
Integration method	Abbreviations	Force evaluations per time step	Extra variables[a]	Accuracy order	
				Position	Velocity
Single-step					
Forward Euler	FE	1	0	1	1
Modified Euler	ME	1	0	2	1
Taylor second order	TY2	1	0	2	1
Taylor third order	TY3	1	1	3	2
Taylor fourth order	TY4	1	2	4	3
Central difference	CD	1	0	2	2
Position Verlet	PV	1	0	2	2
Runge–Kutta fourth order	RK4	4	8	4	4
Multi-step					
Velocity Verlet	VE	1	1	3	2
Adams–Bashforth second order	AB2	1	2	2	2
Adams–Bashforth third order	AB3	1	4	3	3
Adams–Bashforth fourth order	AB4	1	6	4	4
Adams–Bashforth fifth order	AB5	1	8	5	5
Predictor-corrector					
Adams–Moulton third order	AB2AM3	1	5	3	3
Adams–Moulton fourth order	AB3AM4	1	7	4	4
Adams–Moulton fifth order	AB4AM5	1	9	5	5
Gear third order	Gear3	1	4	3	3
Gear fourth order	Gear4	1	5	4	4
Gear fifth order	Gear5	1	6	5	5

Integration of equations (3)



Having time step resolution (α)

$$\Delta t \leq \frac{1}{\alpha} \Delta t_{crit}$$