2016 High Performance Scientific Computing

Register update notification mail

Academic unit or major	Graduate major in Computer Science		
Instructor(s)	Yokota Rio Endo Toshio		
Course component(s)	Lecture		
Day/Period(Room No.)	Thr1-2 Mon1-2		
Group	-		
Course number	CSC.T526	Credits	2
Academic year	2016	Offered quarter	1Q
Syllabus updated	2016/3/28	Lecture notes updated	-
Language used	English	Access Index	★★★★☆

H28年度　高性能科学技術計算　High Performance Scientific Computing

アップデートお知らせメールへ登録

開講元	情報工学コース		
担当教員名	横田 理央 遠藤 敏夫		
授業形態	講義		
曜日・時限(講義室)	木1-2(W831) 月1-2(W831)		
クラス	-		
科目コード	CSC.T526	単位数	2
開講年度	H28年度	開講クォーター	1Q
シラバス更新日	2016年3月28日	講義資料更新日	-
使用言語	英語	アクセスランキング	★★★★☆

		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.

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.

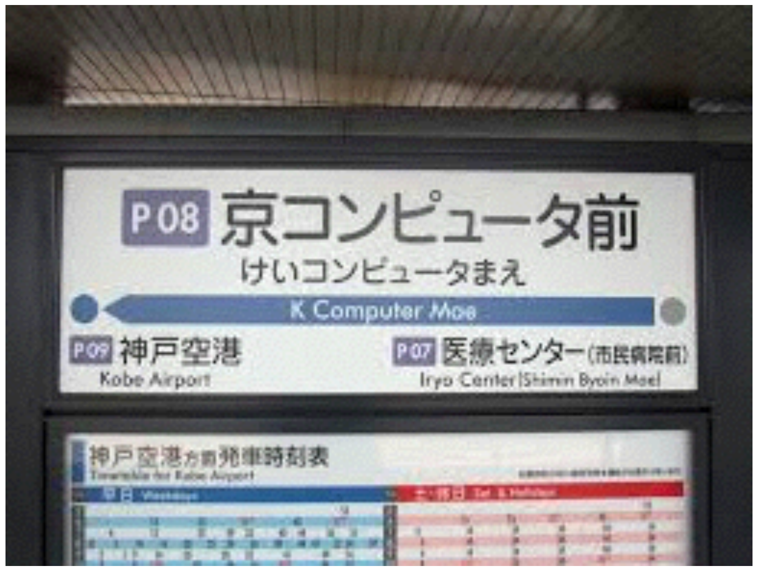
Top500





RANK	SITE	SYSTEM	CORES	RMAX (TFLOP/S)	RPEAK (TFLOP/S)	POWER (KW)
1	National Super Computer Center in Guangzhou China	**Tianhe-2 (MilkyWay-2)** - TH-IVB-FEP Cluster, Intel Xeon E5-2692 12C 2.200GHz, TH Express-2, Intel Xeon Phi 31S1P NUDT	3,120,000	33,862.7	54,902.4	17,808
2	DOE/SC/Oak Ridge National Laboratory United States	**Titan** - Cray XK7 , Opteron 6274 16C 2.200GHz, Cray Gemini interconnect, NVIDIA K20x Cray Inc.	560,640	17,590.0	27,112.5	8,209
3	DOE/NNSA/LLNL United States	**Sequoia** - BlueGene/Q, Power BQC 16C 1.60 GHz, Custom IBM	1,572,864	17,173.2	20,132.7	7,890
4	RIKEN Advanced Institute for Computational Science (AICS) Japan	K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect Fujitsu	705,024	10,510.0	11,280.4	12,660
5	DOE/SC/Argonne National Laboratory United States	**Mira** - BlueGene/Q, Power BQC 16C 1.60GHz, Custom IBM	786,432	8,586.6	10,066.3	3,945
6	DOE/NNSA/LANL/SNL United States	**Trinity** - Cray XC40, Xeon E5-2698v3 16C 2.3GHz, Aries interconnect Cray Inc.	301,056	8,100.9	11,078.9	
7	Swiss National Supercomputing Centre (CSCS) Switzerland	**Piz Daint** - Cray XC30, Xeon E5-2670 8C 2.600GHz, Aries interconnect , NVIDIA K20x Cray Inc.	115,984	6,271.0	7,788.9	2,325
8	HLRS - Höchstleistungsrechenzentrum Stuttgart Germany	**Hazel Hen** - Cray XC40, Xeon E5-2680v3 12C 2.5GHz, Aries interconnect Cray Inc.	185,088	5,640.2	7,403.5	
9	King Abdullah University of Science and Technology Saudi Arabia	**Shaheen II** - Cray XC40, Xeon E5-2698v3 16C 2.3GHz, Aries interconnect Cray Inc.	196,608	5,537.0	7,235.2	2,834

K computer



総開発費1,120億円

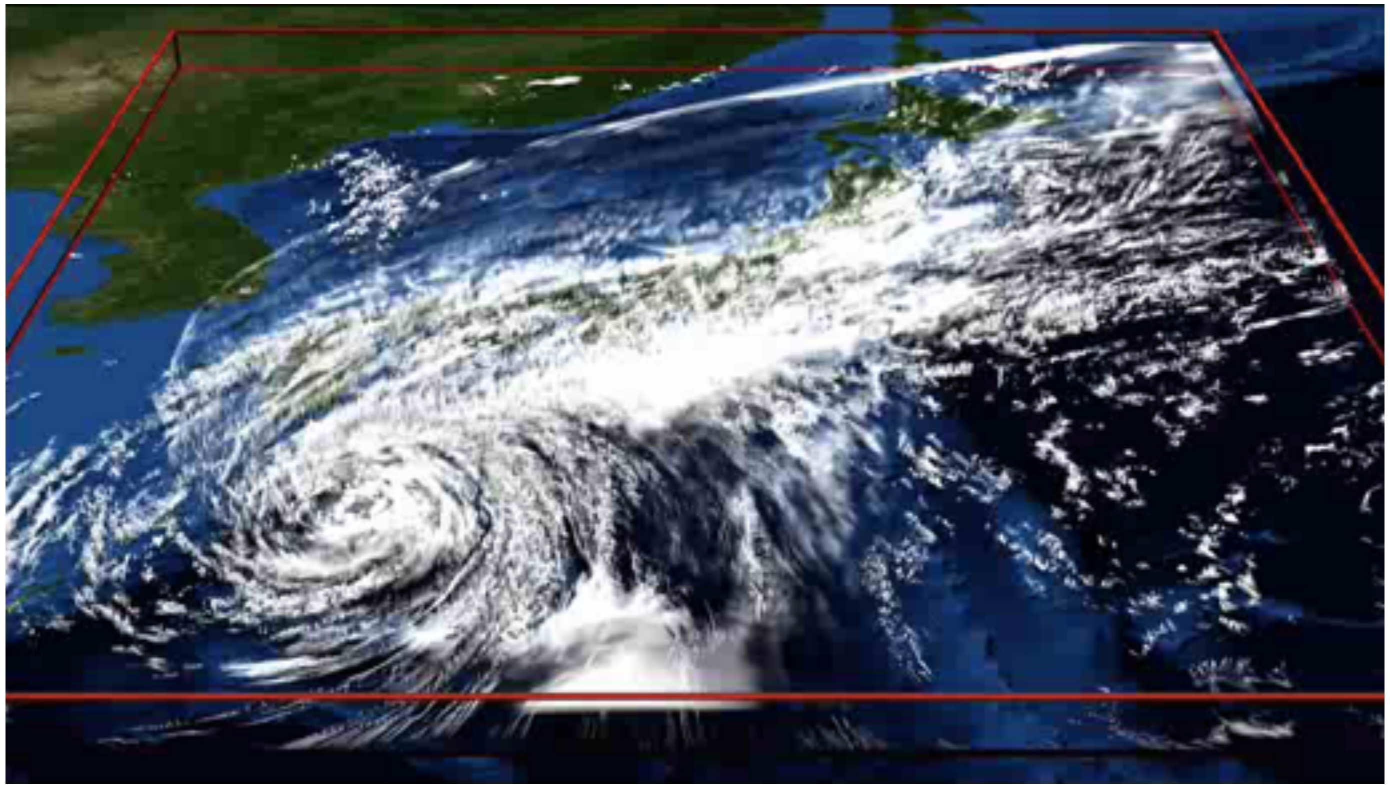
2012年6月に完成

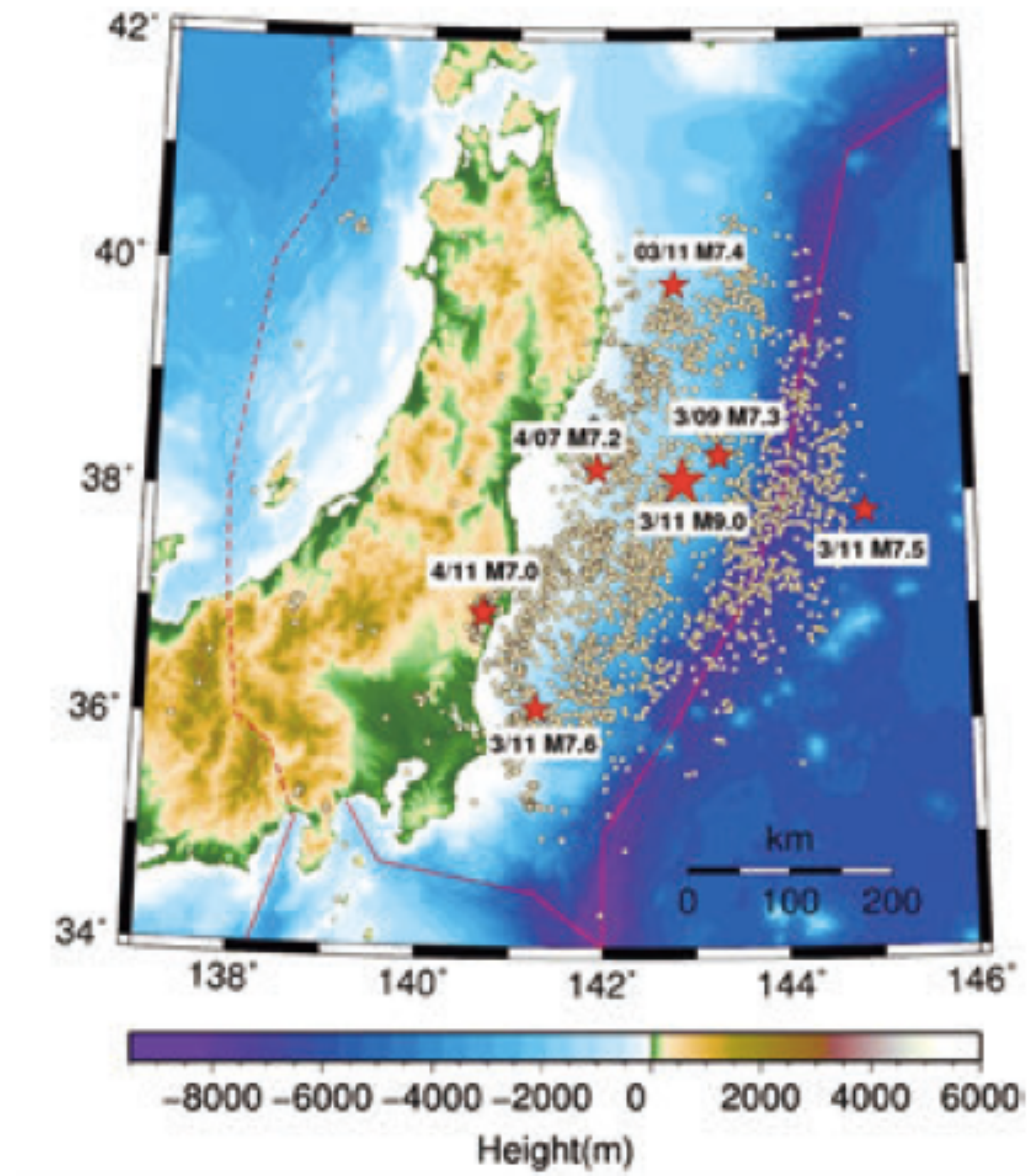
10.5 PFlops

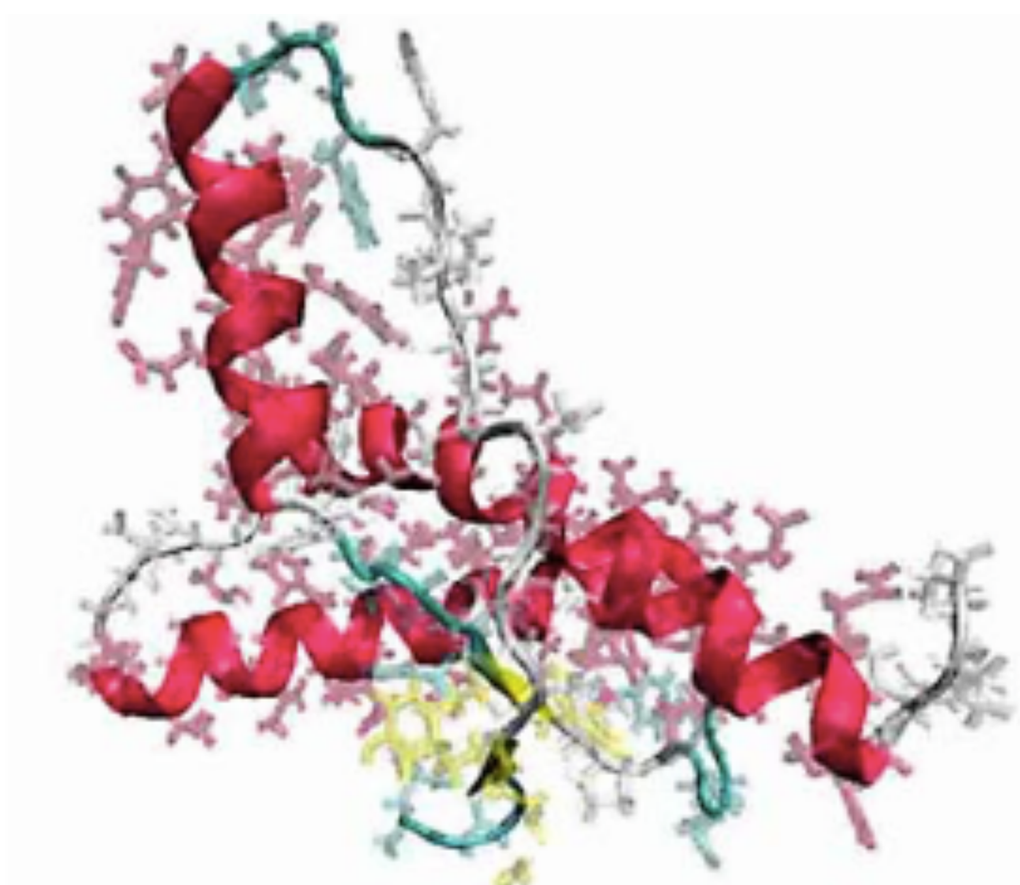
TSUBAME

5.76 PFlops

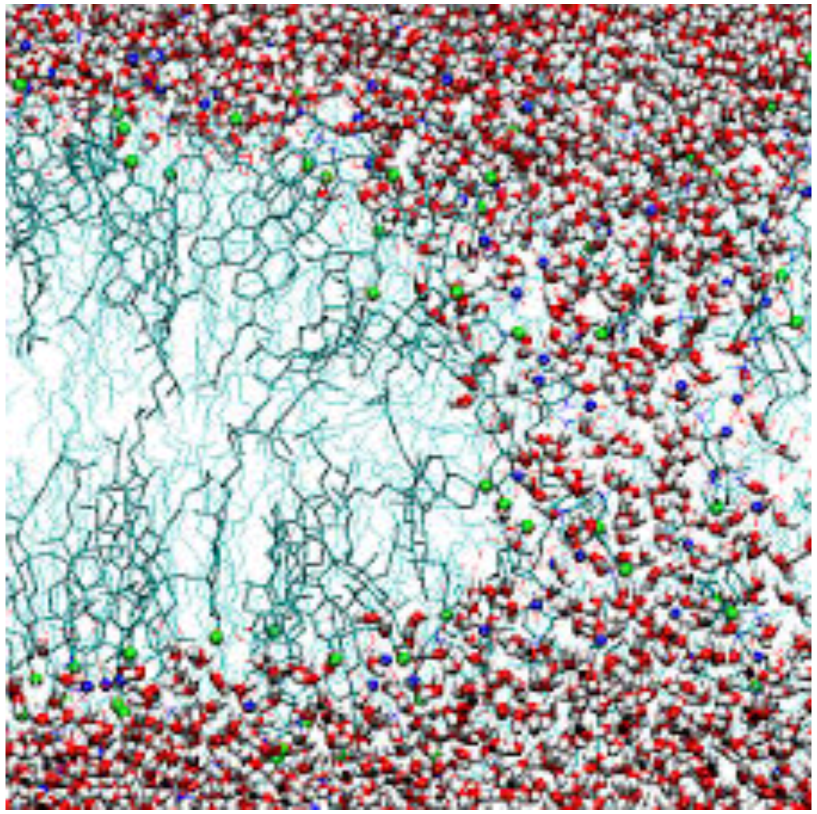
Simulation on TSUBAME

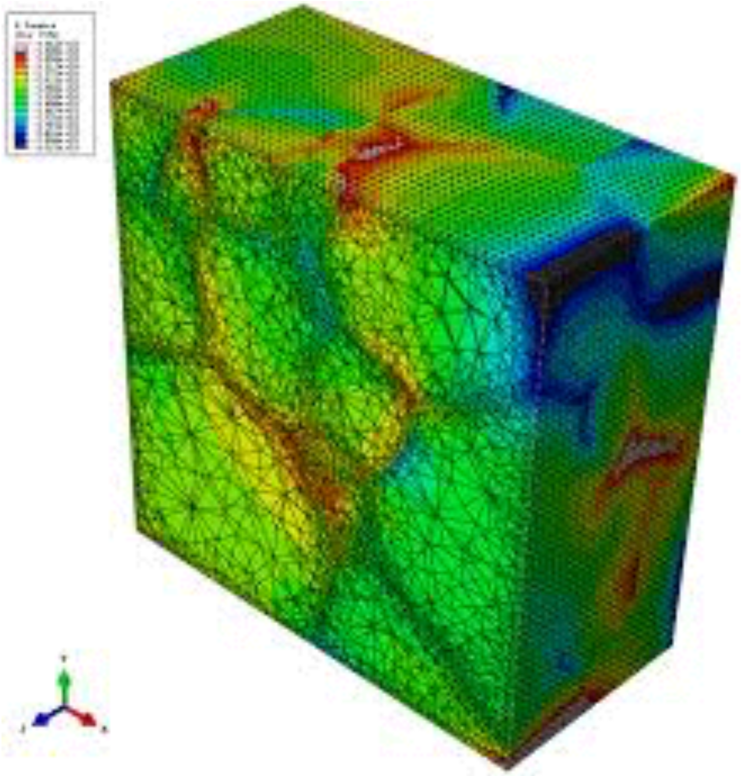


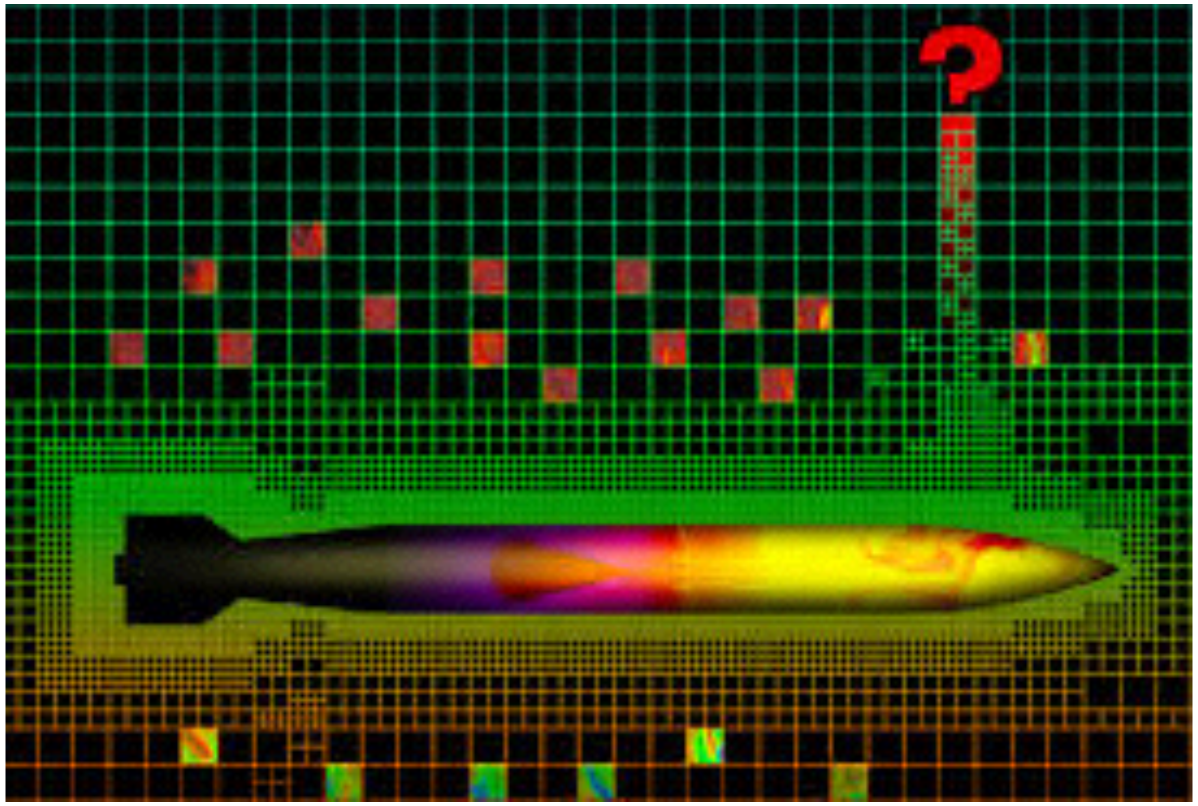


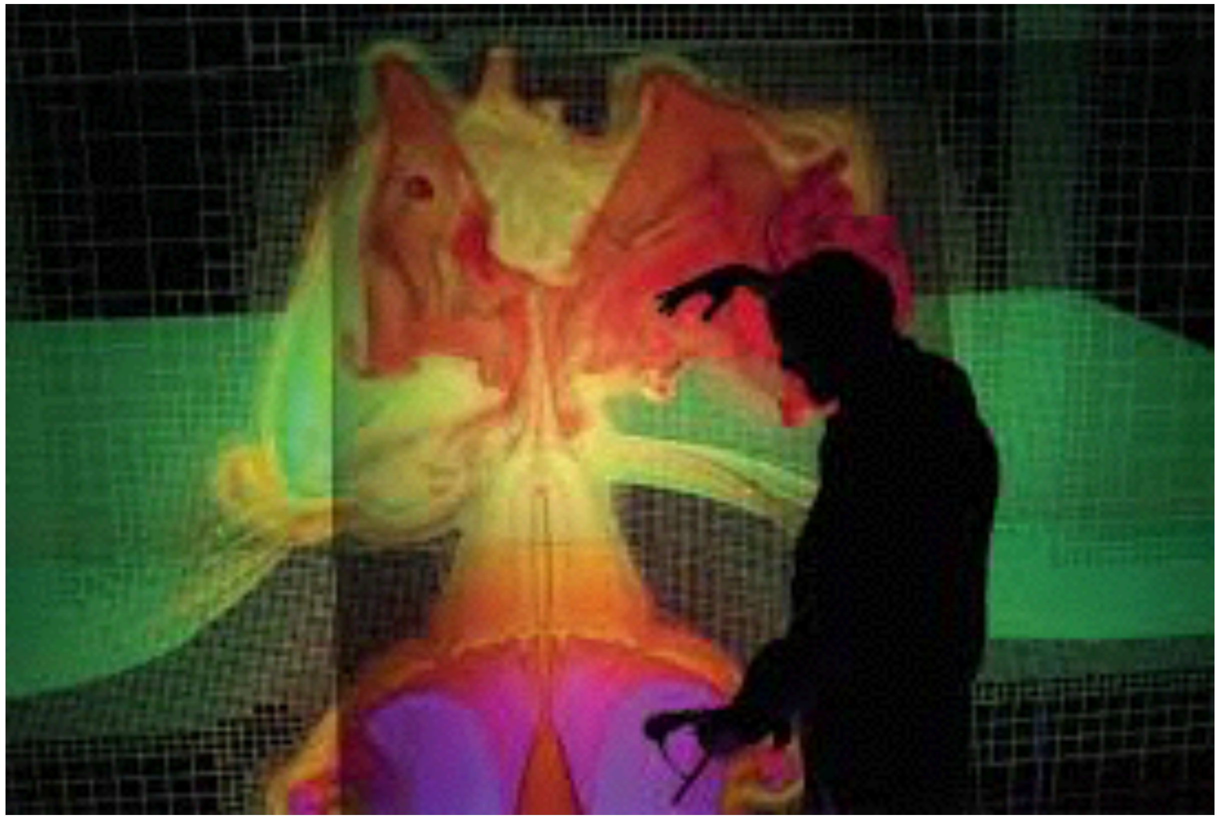


Discretization

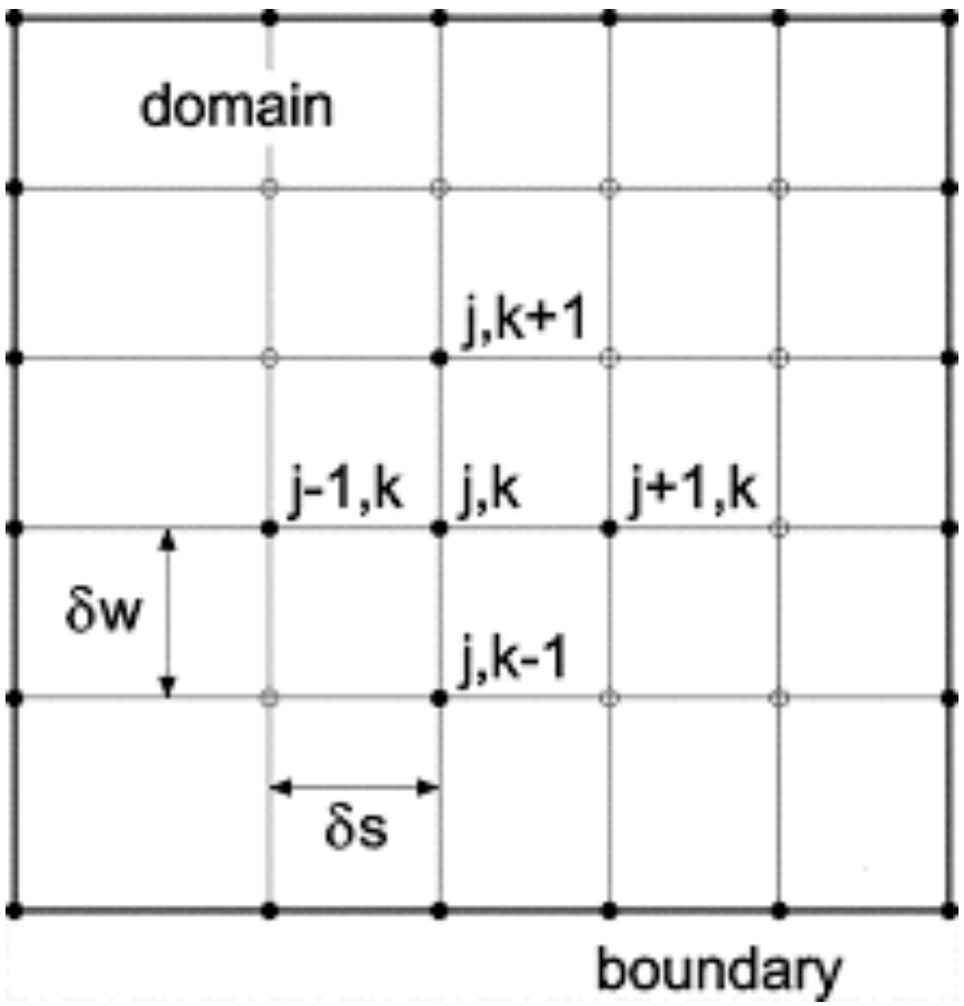






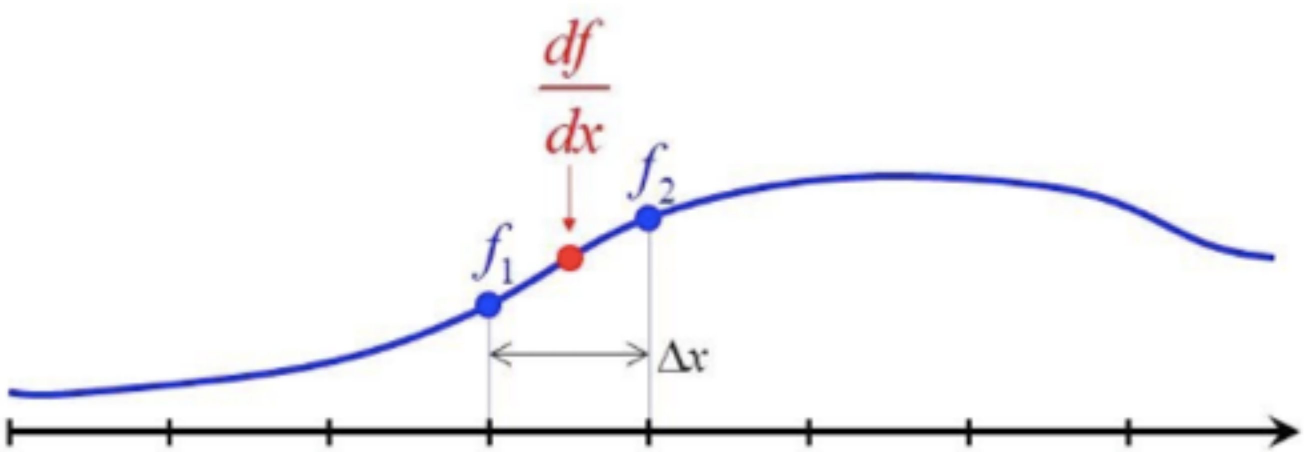


Finite difference methods



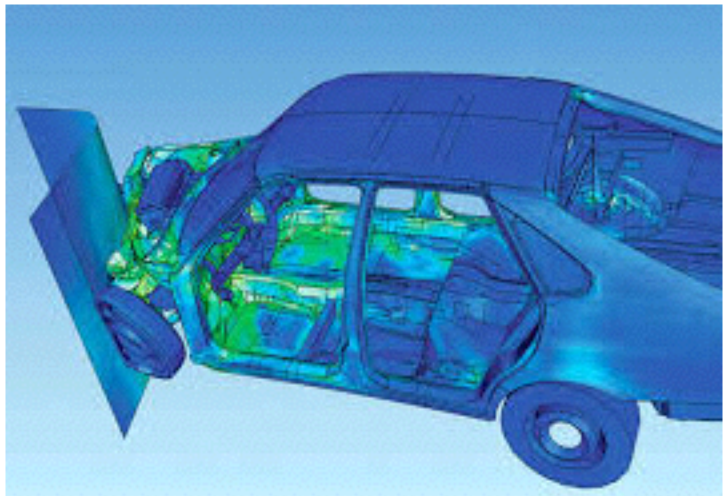
$$\frac{df_{1.5}}{dx} \approx \frac{f_2 - f_1}{\Delta x}$$

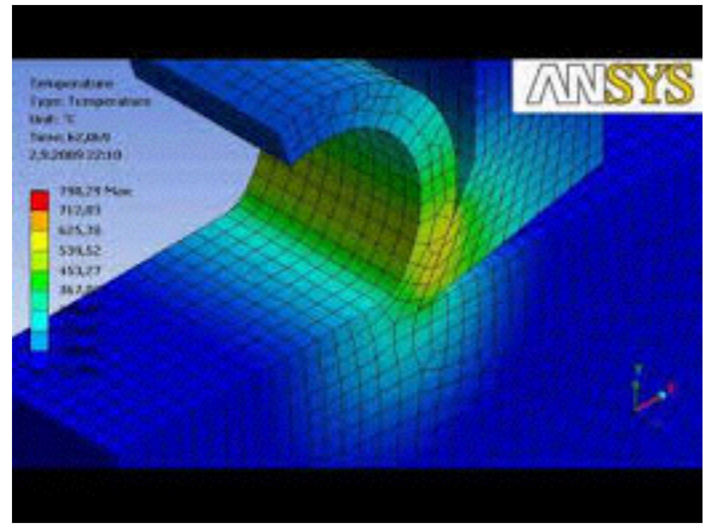
second-order accurate
first-order derivative

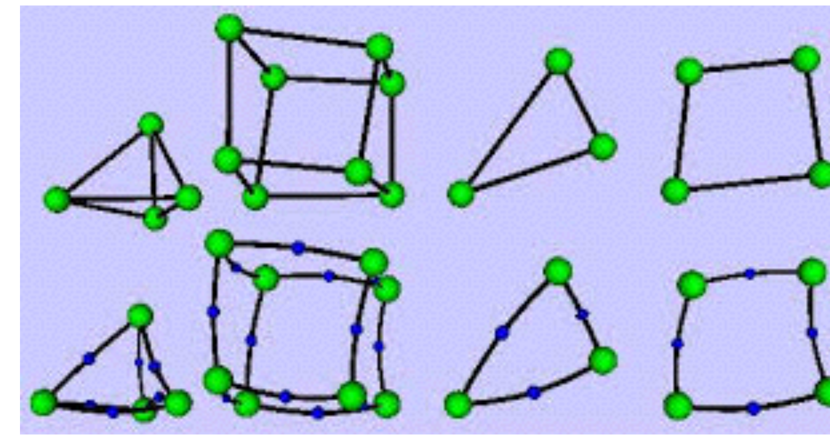


$$\frac{\partial p}{\partial t} + u\frac{\partial p}{\partial x} - D\frac{\partial^2 p}{\partial x^2} = 0$$

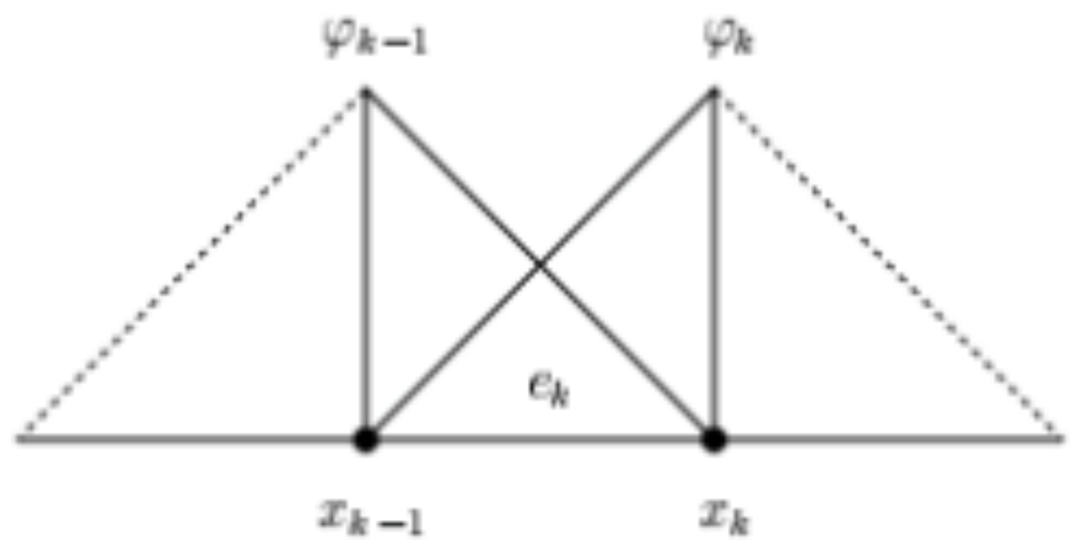
Finite element methods



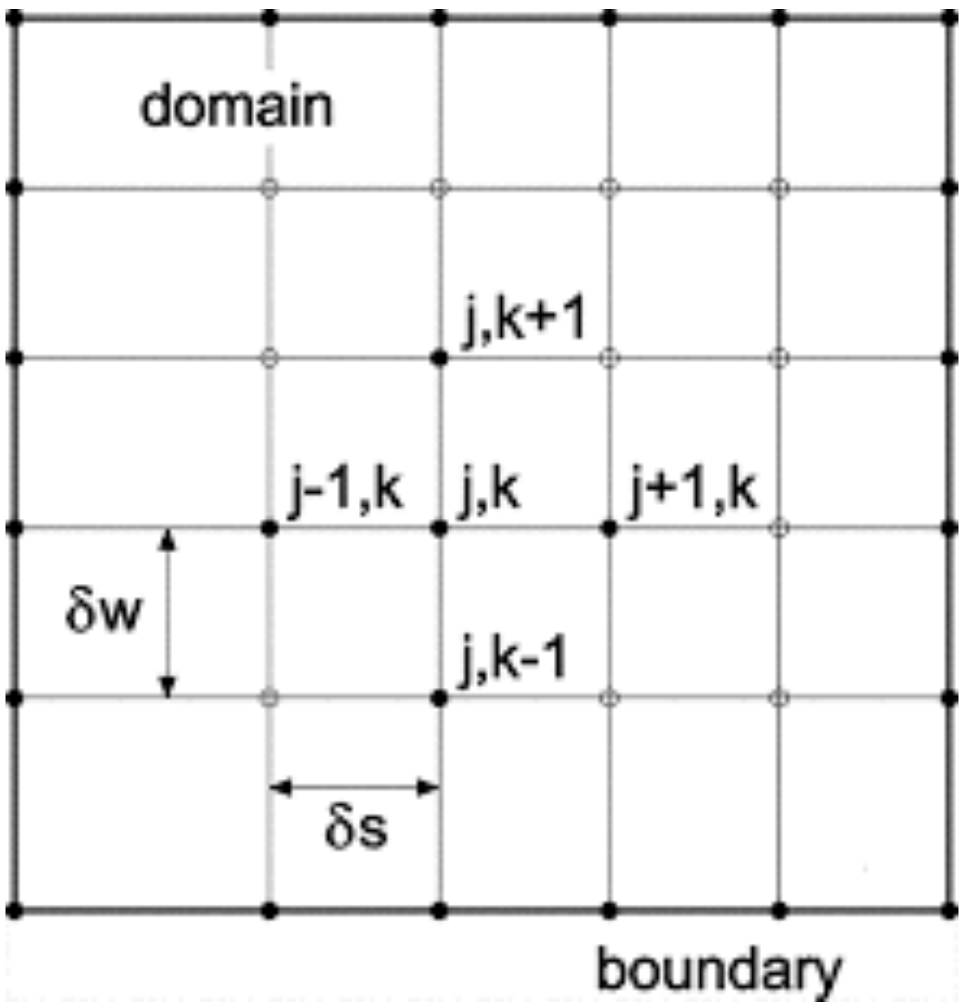




$$\sum_{j=1}^{N} u_j \int_0^1 \frac{d\varphi_i}{dx} \frac{d\varphi_j}{dx}\, dx = \int_0^1 f \varphi_i \, dx,$$

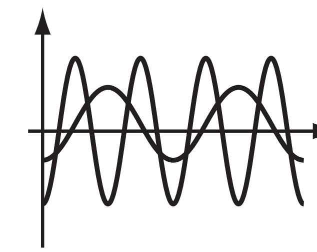


Spectral methods



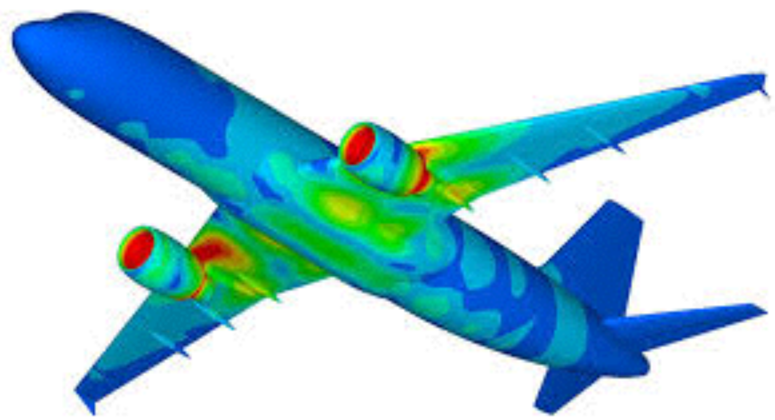
$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) f(x,y) = g(x,y)$$

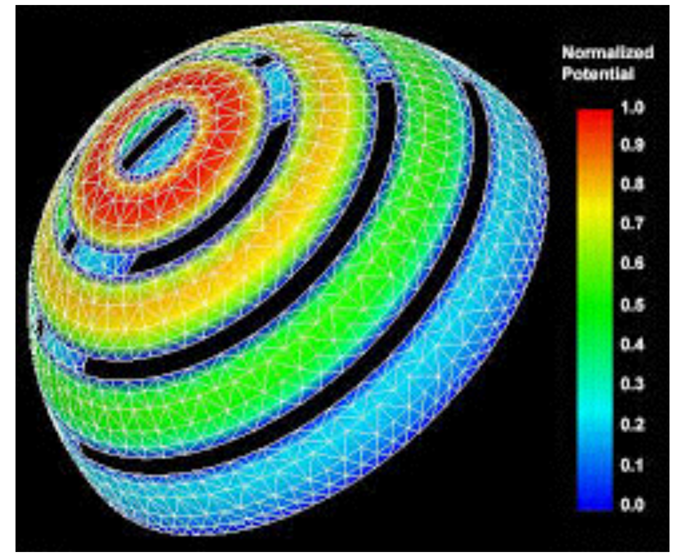
$$f =: \sum a_{j,k} e^{i(jx+ky)}$$
$$g =: \sum b_{j,k} e^{i(jx+ky)}$$



$$\sum -a_{j,k}(j^2 + k^2) e^{i(jx+ky)} = \sum b_{j,k} e^{i(jx+ky)}$$

Boundary element methods

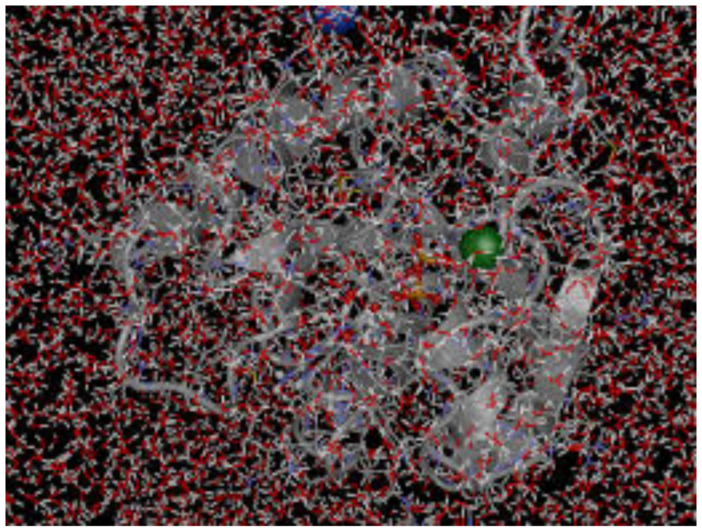


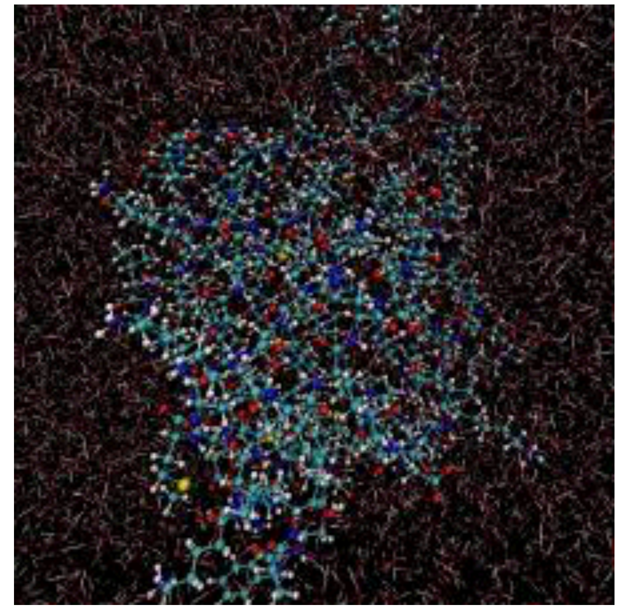


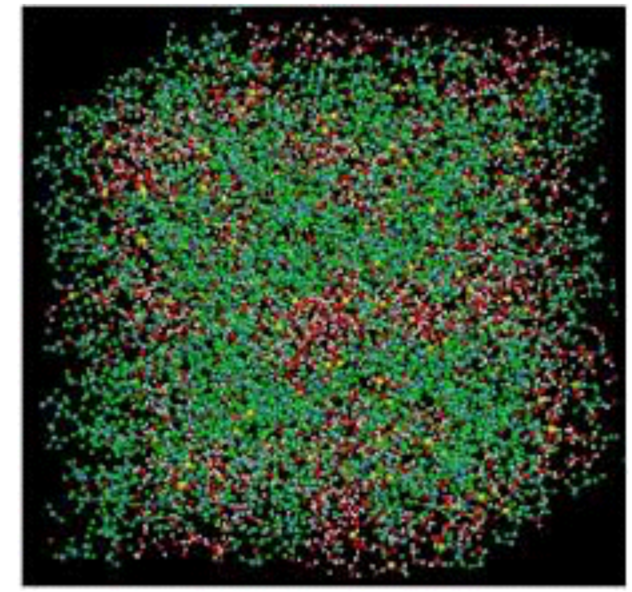
$$\int_{\Omega_b} \left(u^*(\boldsymbol{x},\boldsymbol{x}_0)\nabla^2 u(\boldsymbol{x}) - u(\boldsymbol{x})\nabla^2 u^*(\boldsymbol{x},\boldsymbol{x}_0) \right) d\Omega$$

$$= \int_{\Gamma_b} \left(u^*(\boldsymbol{x},\boldsymbol{x}_0)\frac{\partial u(\boldsymbol{x})}{\partial \boldsymbol{n}} - u(\boldsymbol{x})\frac{\partial u^*(\boldsymbol{x},\boldsymbol{x}_0)}{\partial \boldsymbol{n}} \right) d\Gamma_b(\boldsymbol{x})$$

Molecular dynamics







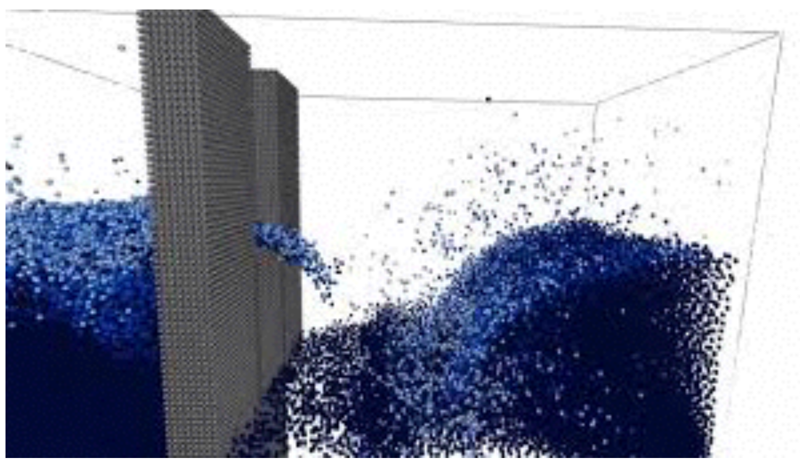
$$V = \sum_{bonds} \frac{1}{2} K_{ij}{}^{b} (r_{ij} - b_{ij})^2 + \sum_{angles} \frac{1}{2} K_{ijk}{}^{\theta} (\theta_{ijk} - \theta_{ijk}{}^{0})^2$$

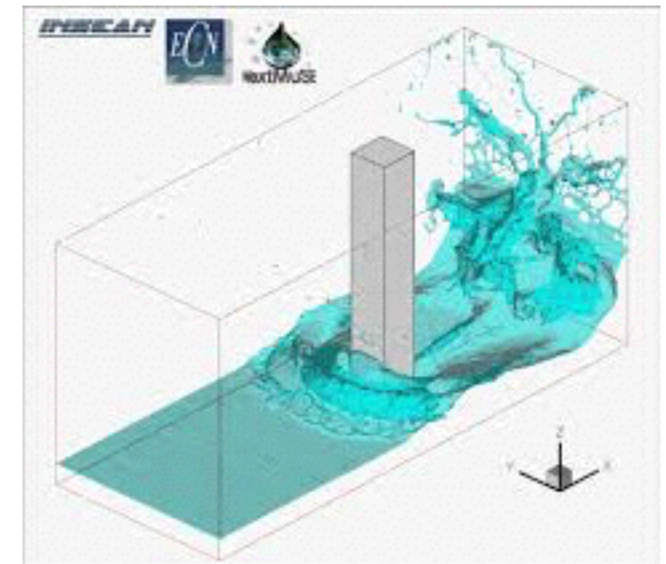
$$+ \sum_{dihedrals} K_{\varphi} (1 + \cos(n\varphi - \varphi_0))$$

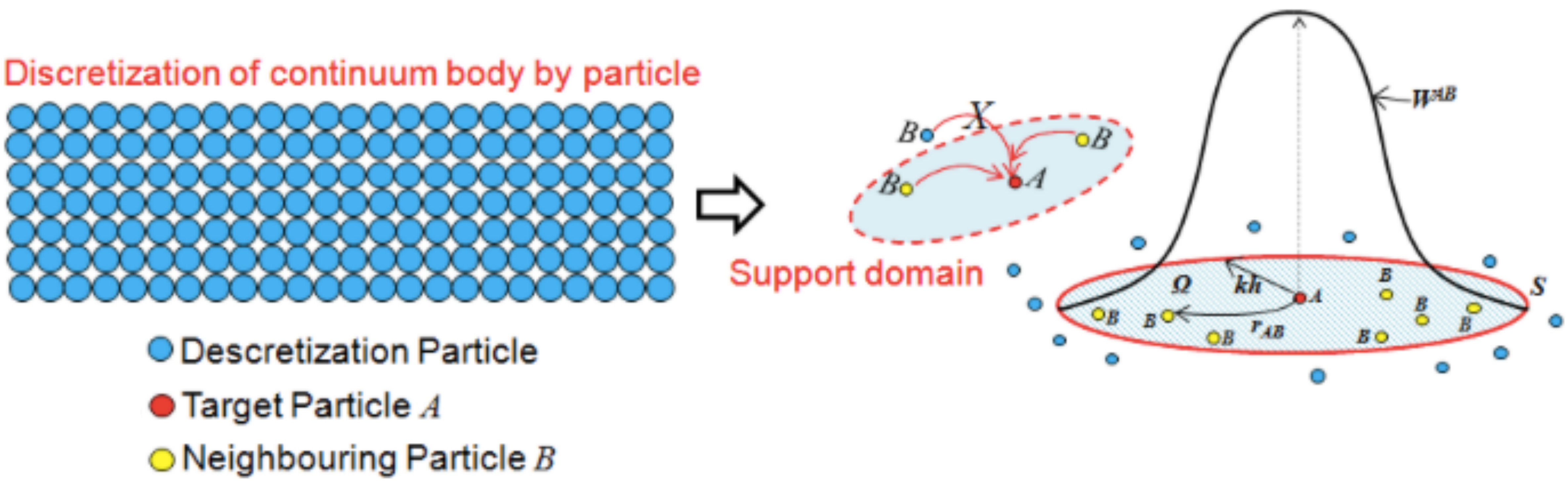
$$+ \sum_{i \neq j} 4\varepsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^{6} \right] + \sum_{i \neq j} \frac{q_i q_j}{\varepsilon_0 r_{ij}}$$

$$\vec{F} = m\vec{a}$$

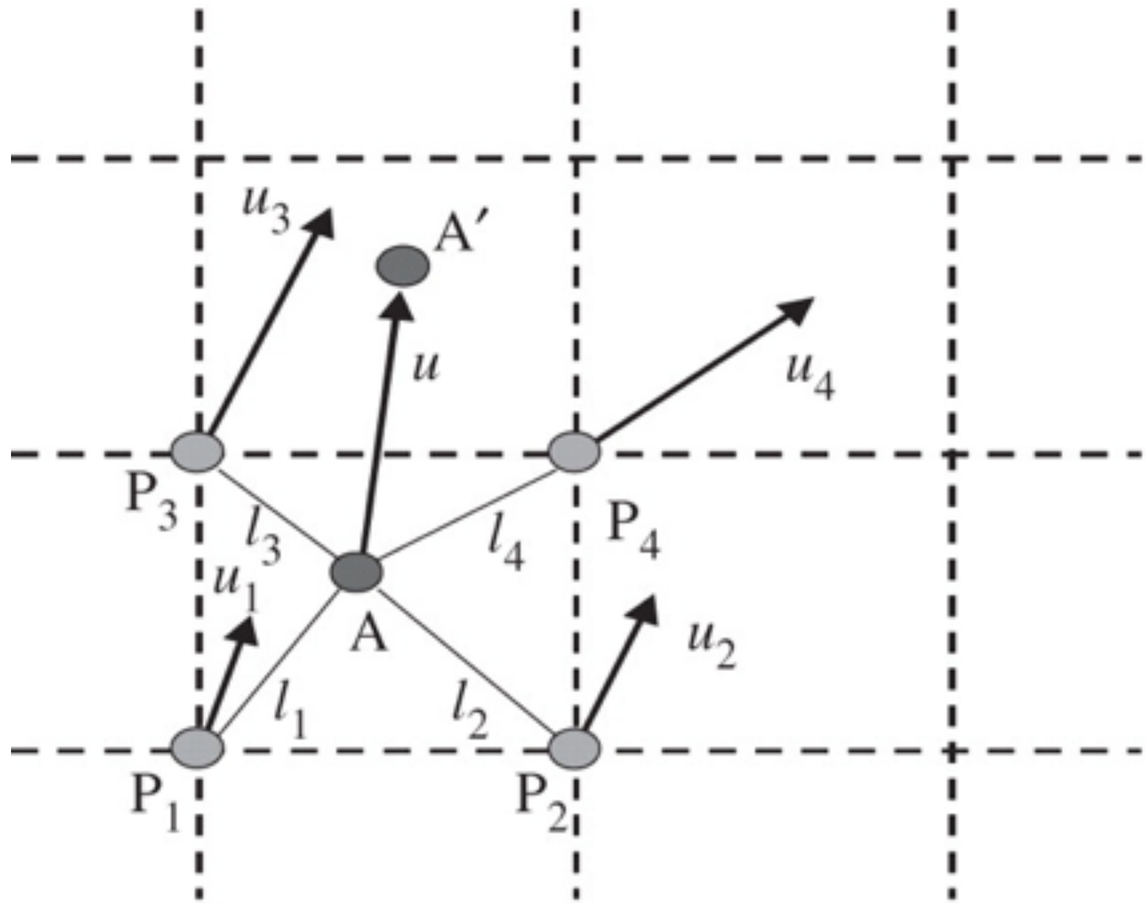
Smooth particle hydrodynamics

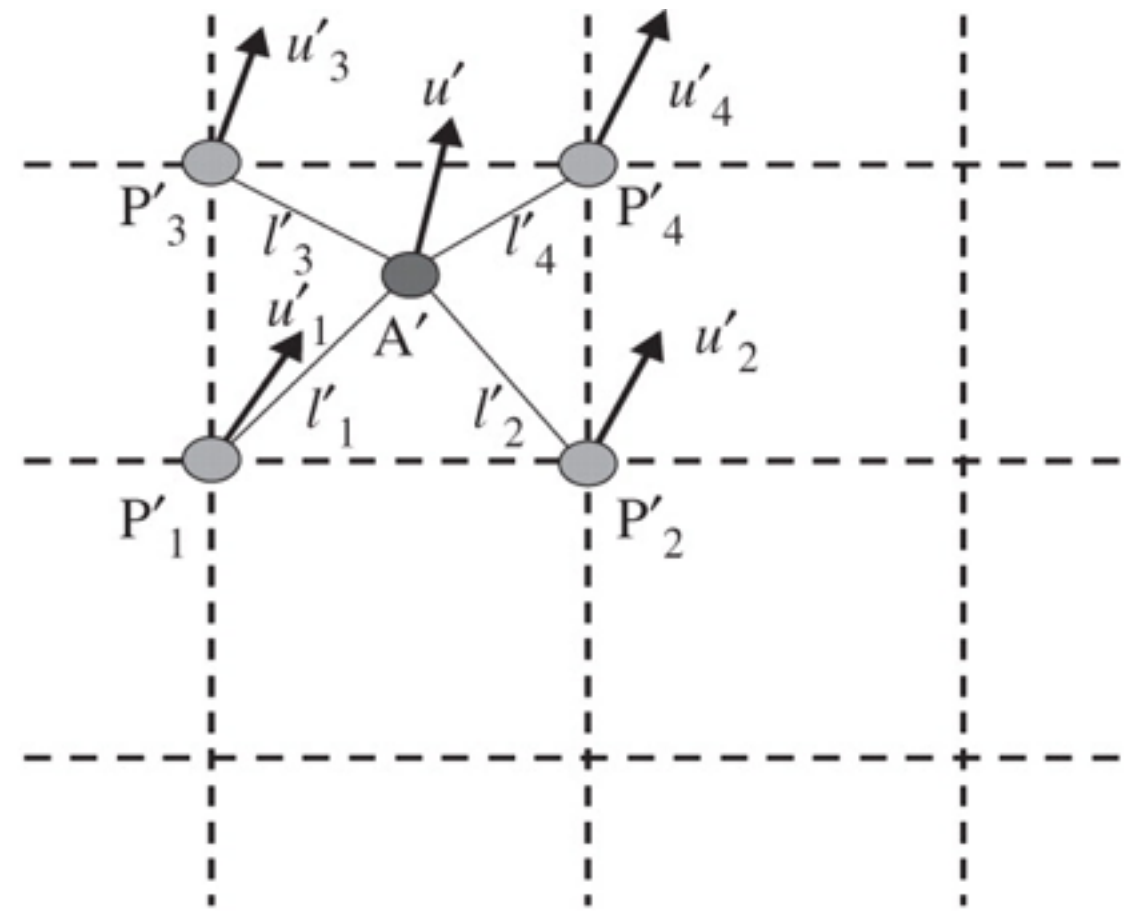






Particle-mesh methods

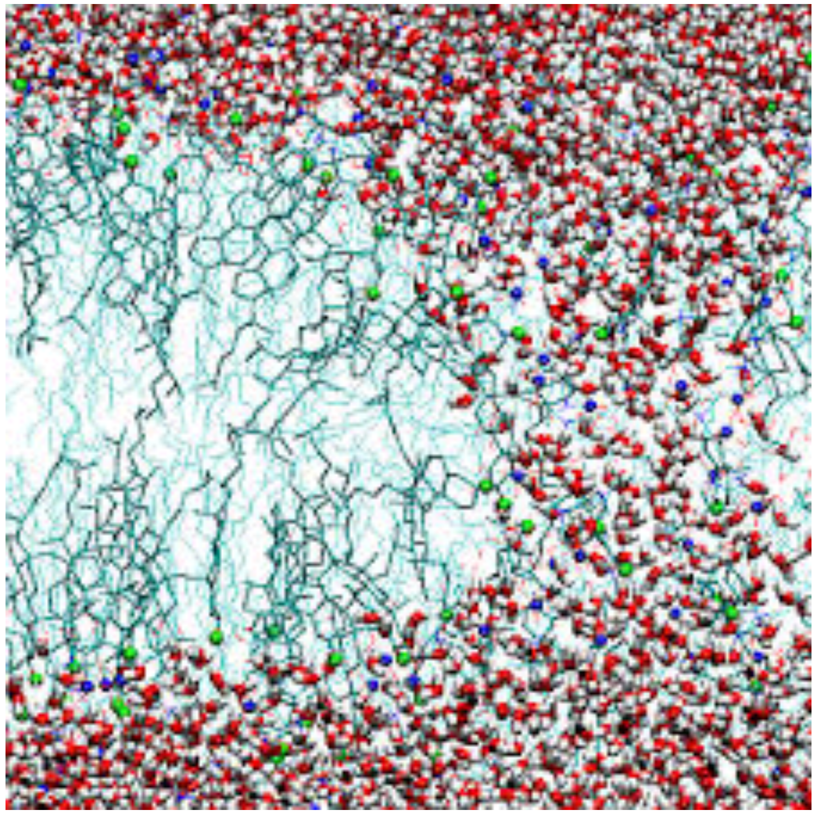


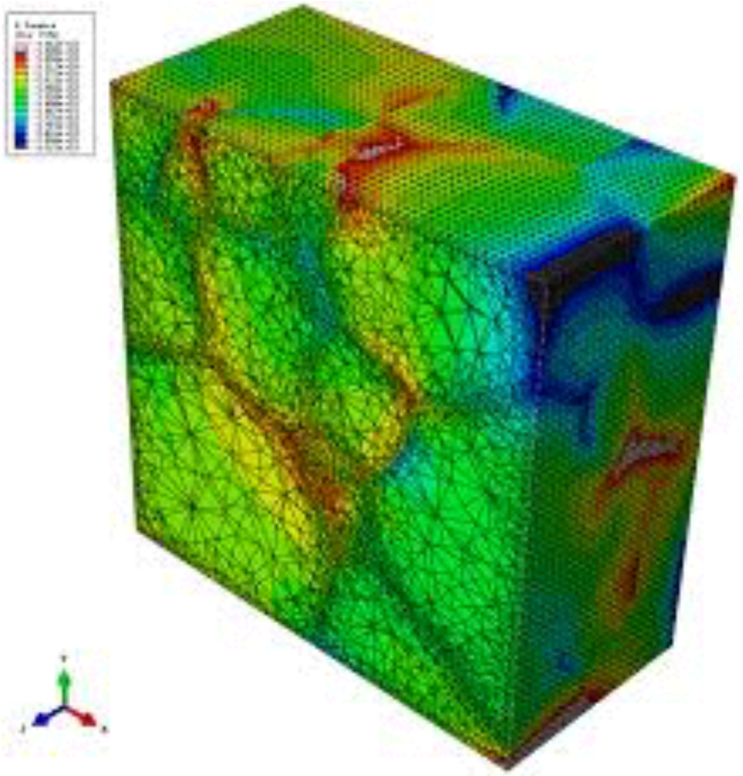


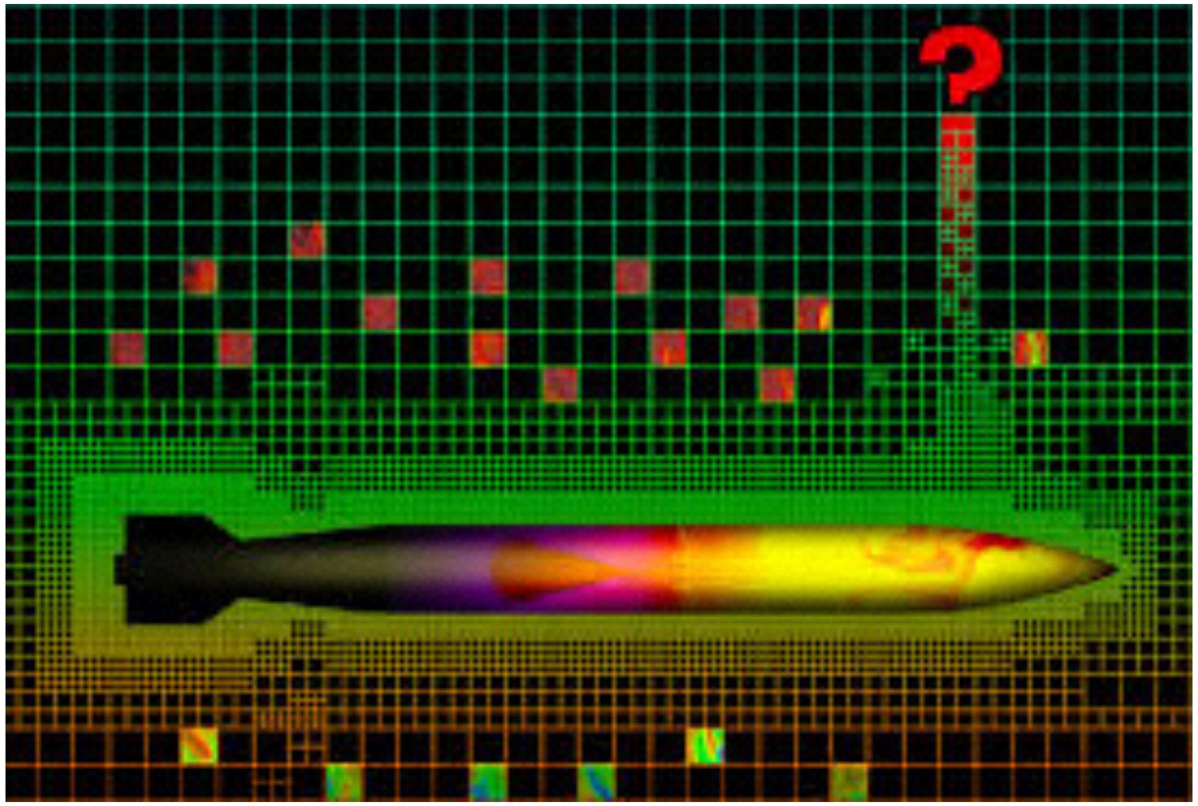
$$u = \frac{\frac{u_1}{l_1} + \frac{u_2}{l_2} + \frac{u_3}{l_3} + \frac{u_4}{l_4}}{\frac{1}{l_1} + \frac{1}{l_2} + \frac{1}{l_3} + \frac{1}{l_4}}$$

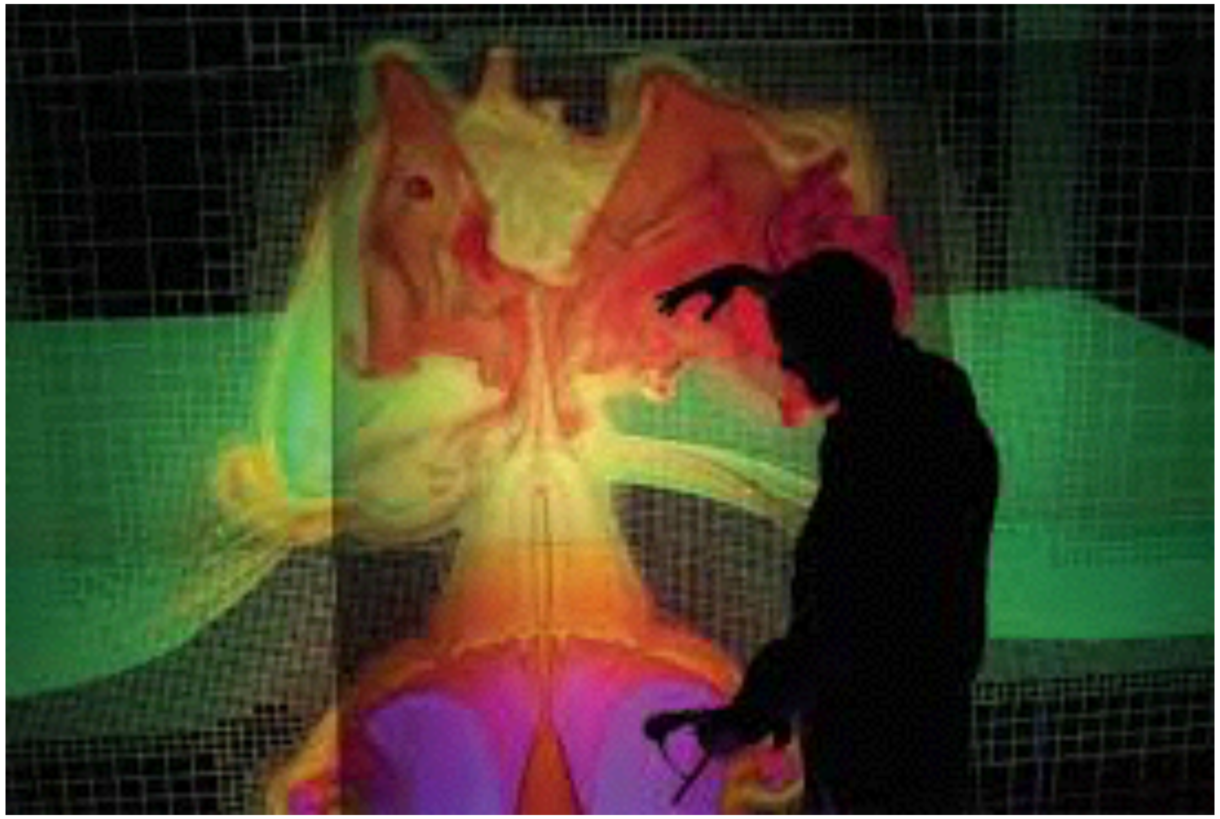
$$u' = \frac{\frac{u'_1}{l'_1} + \frac{u'_2}{l'_2} + \frac{u'_3}{l'_3} + \frac{u'_4}{l'_4}}{\frac{1}{l'_1} + \frac{1}{l'_2} + \frac{1}{l'_3} + \frac{1}{l'_4}}$$

Discretization

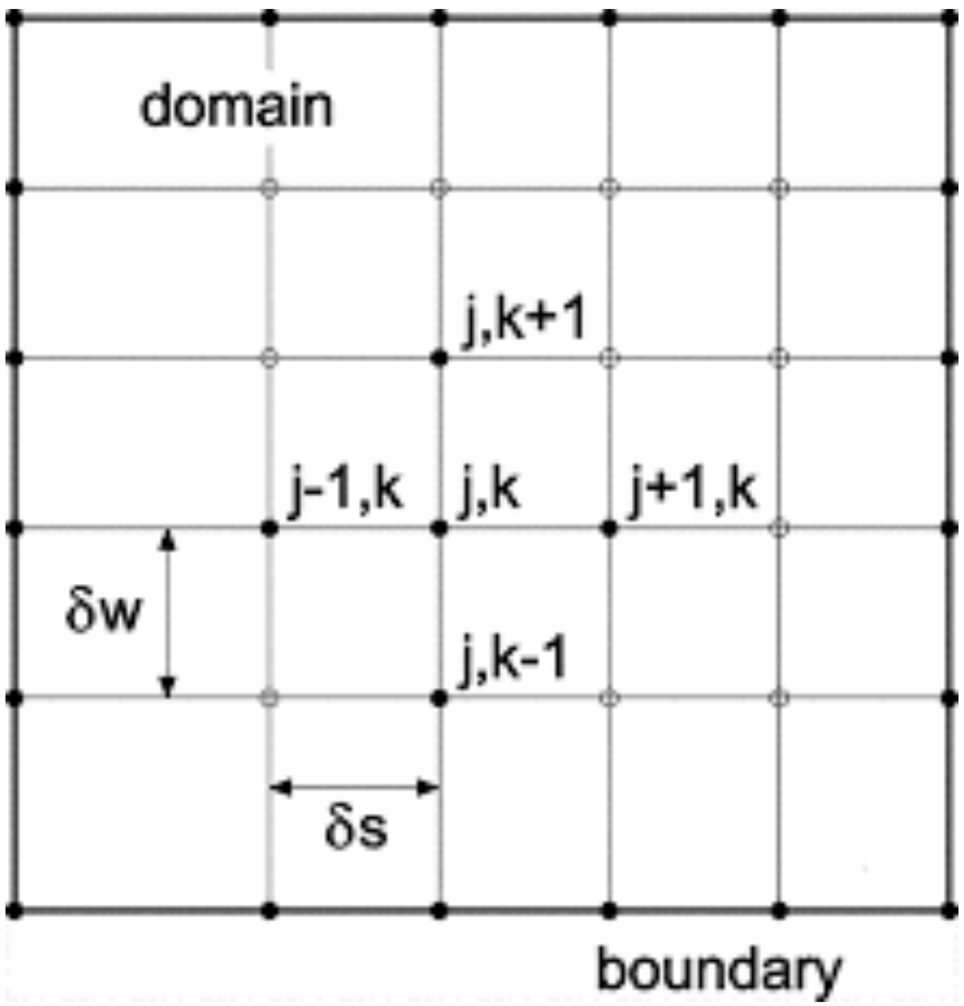






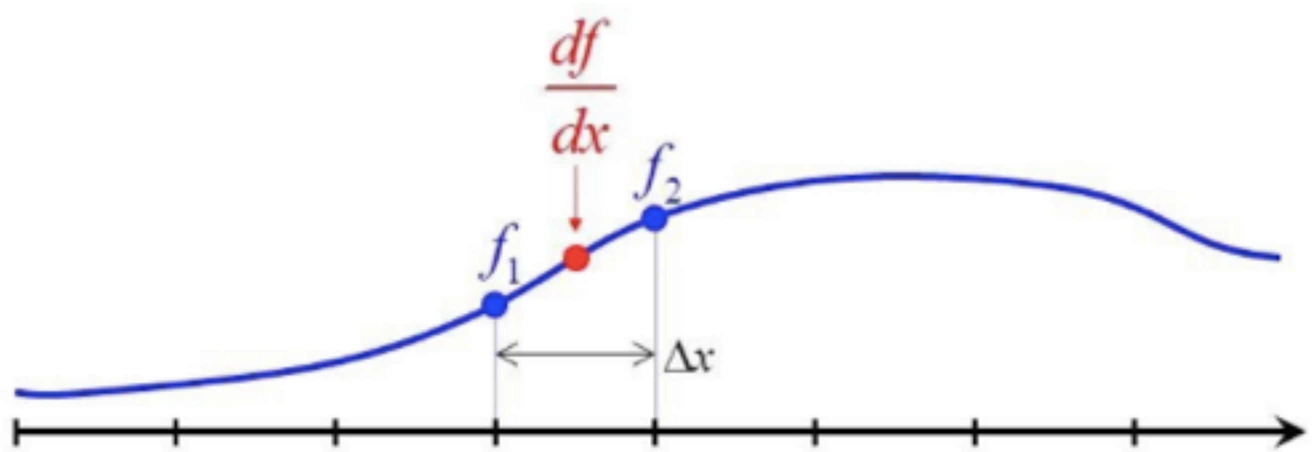


Finite difference methods



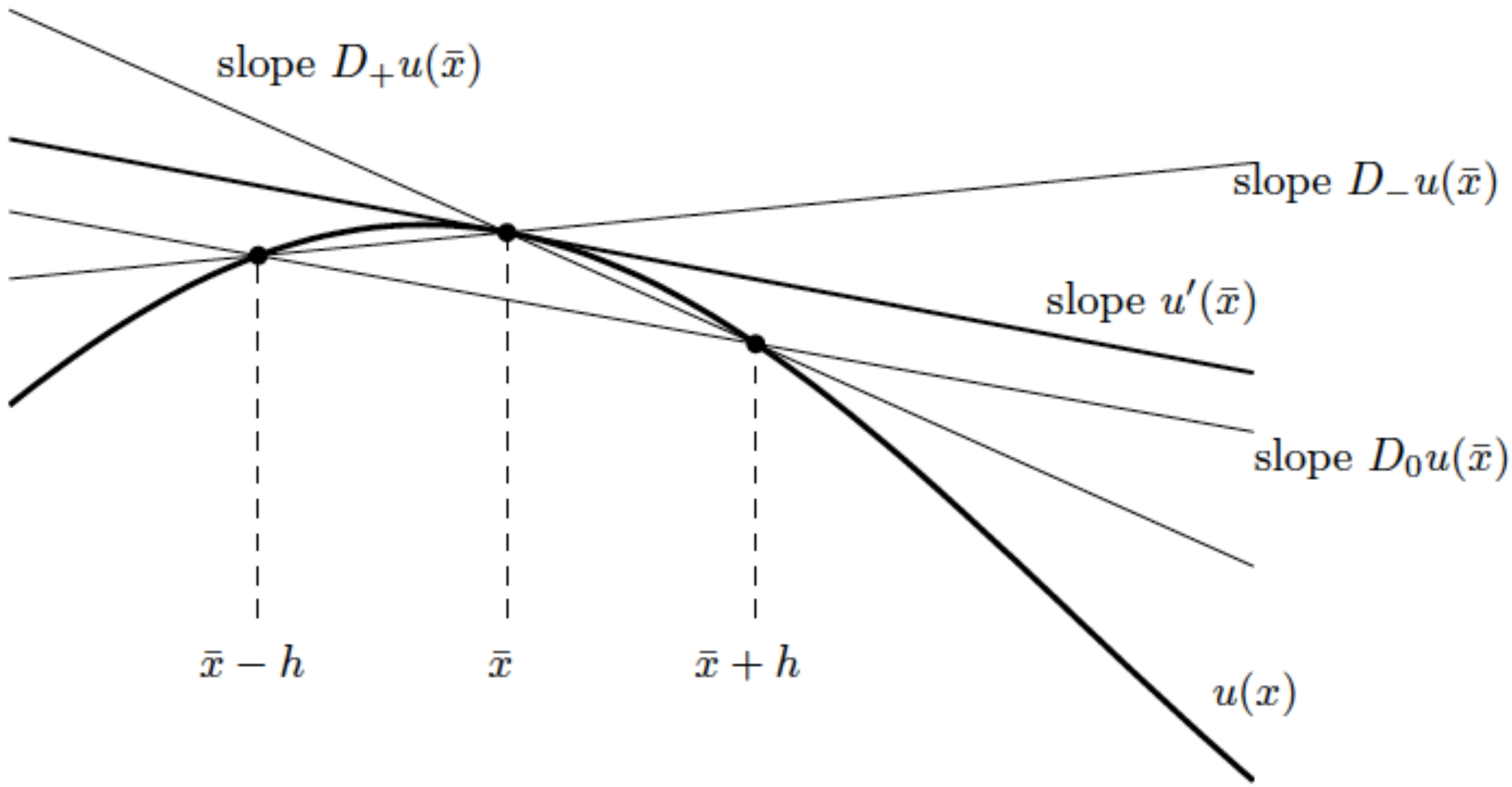
$$\frac{df_{1.5}}{dx} \approx \frac{f_2 - f_1}{\Delta x}$$

second-order accurate
first-order derivative



$$\frac{\partial p}{\partial t} + u\frac{\partial p}{\partial x} - D\frac{\partial^2 p}{\partial x^2} = 0$$

Forward, backward, central difference

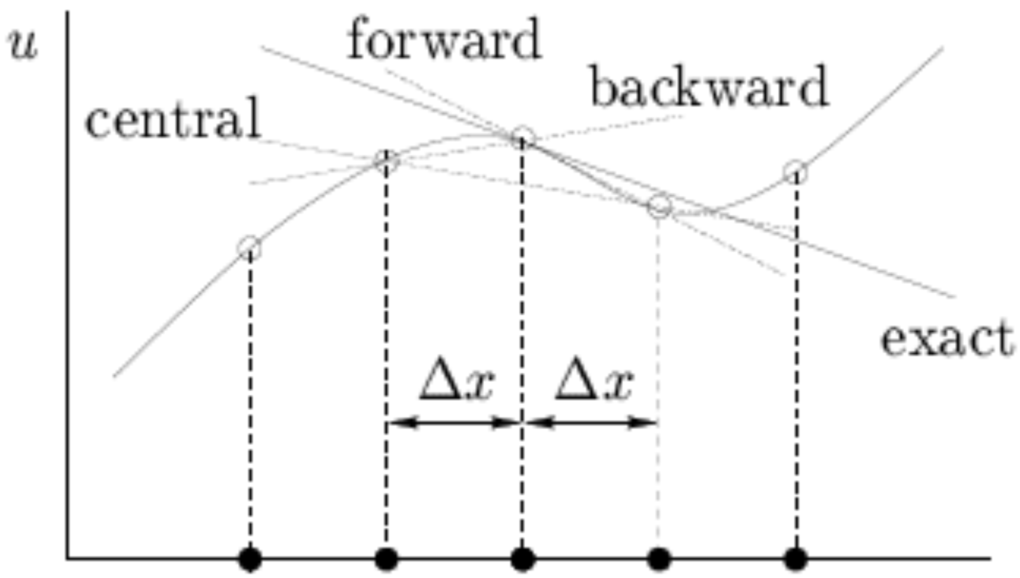


Forward difference $$D_+u(\bar{x}) \equiv \frac{u(\bar{x}+h)-u(\bar{x})}{h}$$

Backward difference $$D_-u(\bar{x}) \equiv \frac{u(\bar{x})-u(\bar{x}-h)}{h}$$

Central difference $$D_0u(\bar{x}) \equiv \frac{u(\bar{x}+h)-u(\bar{x}-h)}{2h} = \frac{1}{2}(D_+u(\bar{x})+D_-u(\bar{x}))$$

Truncation error



$$\left(\frac{\partial u}{\partial x}\right)_i \approx \frac{u_{i+1}-u_i}{\Delta x} \qquad \text{forward difference}$$

$$\left(\frac{\partial u}{\partial x}\right)_i \approx \frac{u_i-u_{i-1}}{\Delta x} \qquad \text{backward difference}$$

$$\left(\frac{\partial u}{\partial x}\right)_i \approx \frac{u_{i+1}-u_{i-1}}{2\Delta x} \qquad \text{central difference}$$

$$T_1 \quad \Rightarrow \quad \left(\frac{\partial u}{\partial x}\right)_i = \frac{u_{i+1}-u_i}{\Delta x} - \frac{\Delta x}{2}\left(\frac{\partial^2 u}{\partial x^2}\right)_i - \frac{(\Delta x)^2}{6}\left(\frac{\partial^3 u}{\partial x^3}\right)_i + \dots$$

forward difference truncation error $\mathcal{O}(\Delta x)$

$$T_2 \quad \Rightarrow \quad \left(\frac{\partial u}{\partial x}\right)_i = \frac{u_i-u_{i-1}}{\Delta x} + \frac{\Delta x}{2}\left(\frac{\partial^2 u}{\partial x^2}\right)_i - \frac{(\Delta x)^2}{6}\left(\frac{\partial^3 u}{\partial x^3}\right)_i + \dots$$

backward difference truncation error $\mathcal{O}(\Delta x)$

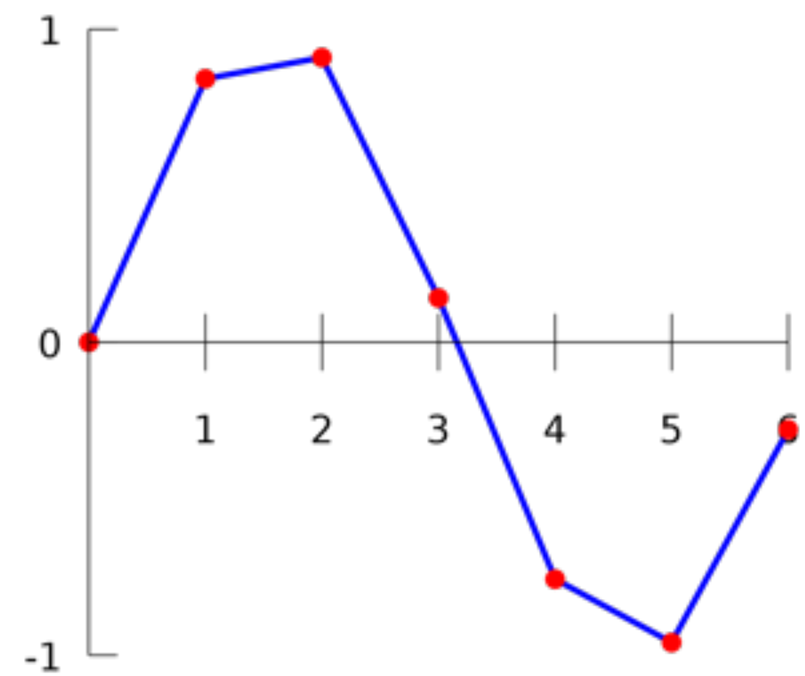
$$T_1 - T_2 \quad \Rightarrow \quad \left(\frac{\partial u}{\partial x}\right)_i = \frac{u_{i+1}-u_{i-1}}{2\Delta x} - \frac{(\Delta x)^2}{6}\left(\frac{\partial^3 u}{\partial x^3}\right)_i + \dots$$

central difference truncation error $\mathcal{O}(\Delta x)^2$

Second order derivative

Consider once more the Taylor series

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f^{(3)}(x) + \frac{h^4}{24}f^{(4)}(\xi)$$
$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f^{(3)}(x) + \frac{h^4}{24}f^{(4)}(\eta)$$



Adding and rearranging terms we obtain

$$\frac{f(x+h) - 2f(x) + f(x-h)}{h^2} = f''(x) + e^h(x)$$

Alternatively, we can use forward and backward approximations:

$$f''(x) \xrightarrow{\text{fwd.}} \frac{f'(x+h) - f'(x)}{h} \xrightarrow{\text{bwd.}} \frac{\frac{f(x+h)-f(x)}{h} - \frac{f(x)-f(x-h)}{h}}{h}$$
$$= \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$

or the other way around

$$f''(x) \xrightarrow{\text{bwd.}} \frac{f'(x) - f'(x-h)}{h} \xrightarrow{\text{fwd.}} \frac{\frac{f(x+h)-f(x)}{h} - \frac{f(x)-f(x-h)}{h}}{h}$$
$$= \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$

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