

H29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	<u>横田 理央</u> <u>遠藤 敏夫</u>		
授業形態	講義		
曜日・時限(講義室)	月1-2(W831) 木1-2(W831)		
クラス	-	単位数	2
科目コード	CSC.T526	開講クォーター	1Q
開講年度	H29年度	講義資料更新日	-
シラバス更新日	H29年3月17日	アクセスランキング	
使用言語	日本語		

	授業計画	課題
04/06	第1回 微分方程式の離散化	前進・後退・中心差分, 高次の差分を用いて微分方程式を離散化し, 誤差を評価できる
04/10	第2回 有限差分法	時間積分の安定性や高次精度の積分を理解し移流・拡散・波動方程式を解析できる
04/13	第3回 有限要素法	Galerkin 法, テスト関数, isoparametric 要素の概念を理解し, 弾性方程式を解析できる
04/17	第4回 スペクトル法	Fourier・Chebyshev・Legendre・Bessel などの直交基底関数による離散化の利点を説明できる
04/20	第5回 境界要素法	逆行列と δ 関数・Green 関数の関係を理解し境界積分方程式を用いた解析ができる
04/24	第6回 分子動力学法	時間積分の symplectic 性や熱浴の概念を理解し分子間に働く保存力の動力学を解析できる
04/27	第7回 Smooth particle hydrodynamics (SPH) 法	微分演算子の動径基底関数による離散化とその保存性・散逸性を評価できる
05/01	第8回 Particle mesh 法	粒子と格子の両方の離散化を組み合わせる場合の離散点からの補間法と高次モーメントの保存法

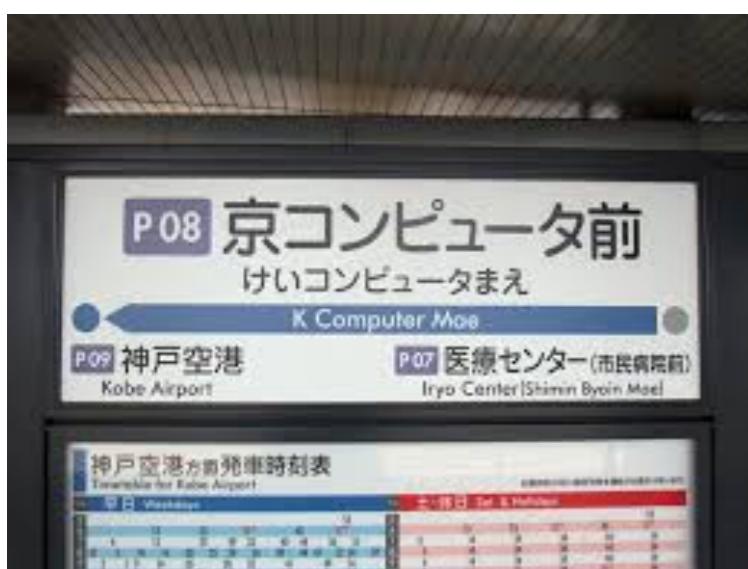
	授業計画	課題
05/08	第9回 密行列の直接解法	LU 分解の原理を理解し、その最適化・並列化と LINPACK ベンチマークの特徴を理解できる
05/11	第10回 密行列の固有値解析	固有値・固有ベクトルの求め方を習得し対角化正規直交化の高速化手法を理解できる
05/15	第11回 疎行列の直接解法	AMD や Nested dissection などの並べ替え法と skyline・multifrontal 法の高速化手法を理解
05/18	第12回 疎行列の反復解法	正定値行列や条件数の概念を理解し、Jacobi 法 CG 法, GMRES 法の相違点を理解
05/22	第13回 反復法の前処理	前処理による条件数やスペクトル半径への影響や前処理された CG 法の効果を理解できる
05/25	第14回 マルチグリッド法	V-cycle における緩和・縮約・補間の役割を理解し前処理法としての効果を理解できる
05/29	第15回 FMM, H 行列	多重極展開、低ランク近似の概念を理解し木構造の果たす役割を理解できる

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	17,308
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 BGC 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	12,560
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



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TSUBAME

東京工業大学 学術国際情報センター

〒152-8550 東京都目黒区大岡山 2-12-1

Phone: (03)5734-2087

FAX: (03)5734-3198

E-mail: office@gsic.titech.ac.jp



緑が丘地区

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北地区

大岡山西地区

学術国際情報センター 情報棟

- ・スパコン 'TSUBAME'
- ・会議室
- ・事務室

正門

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大岡山南地区

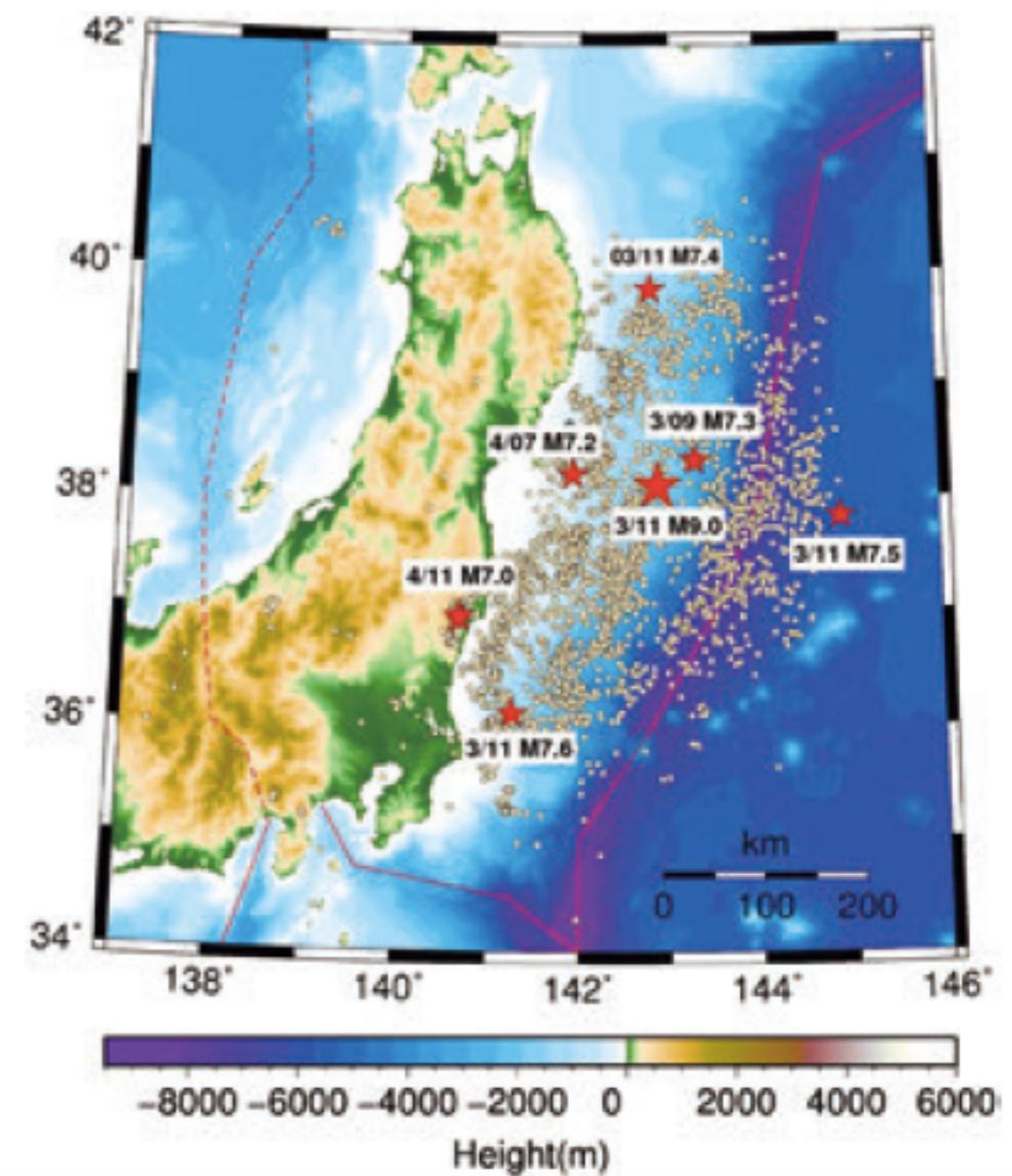
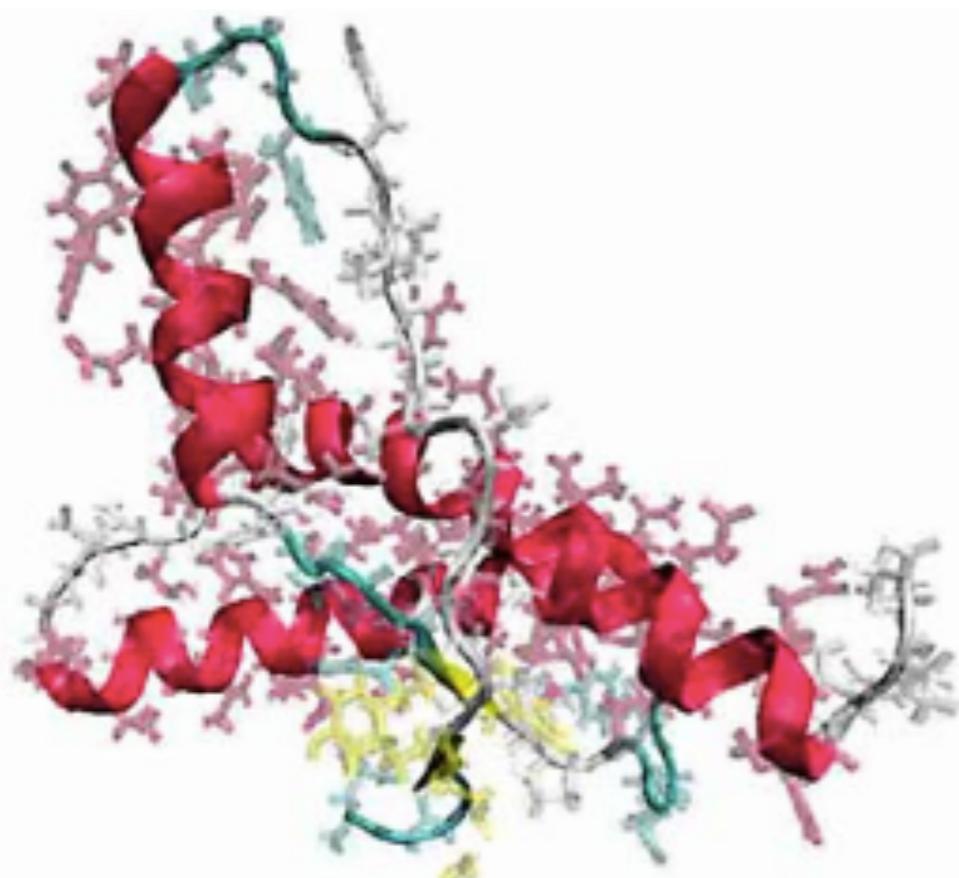
大岡山東地区



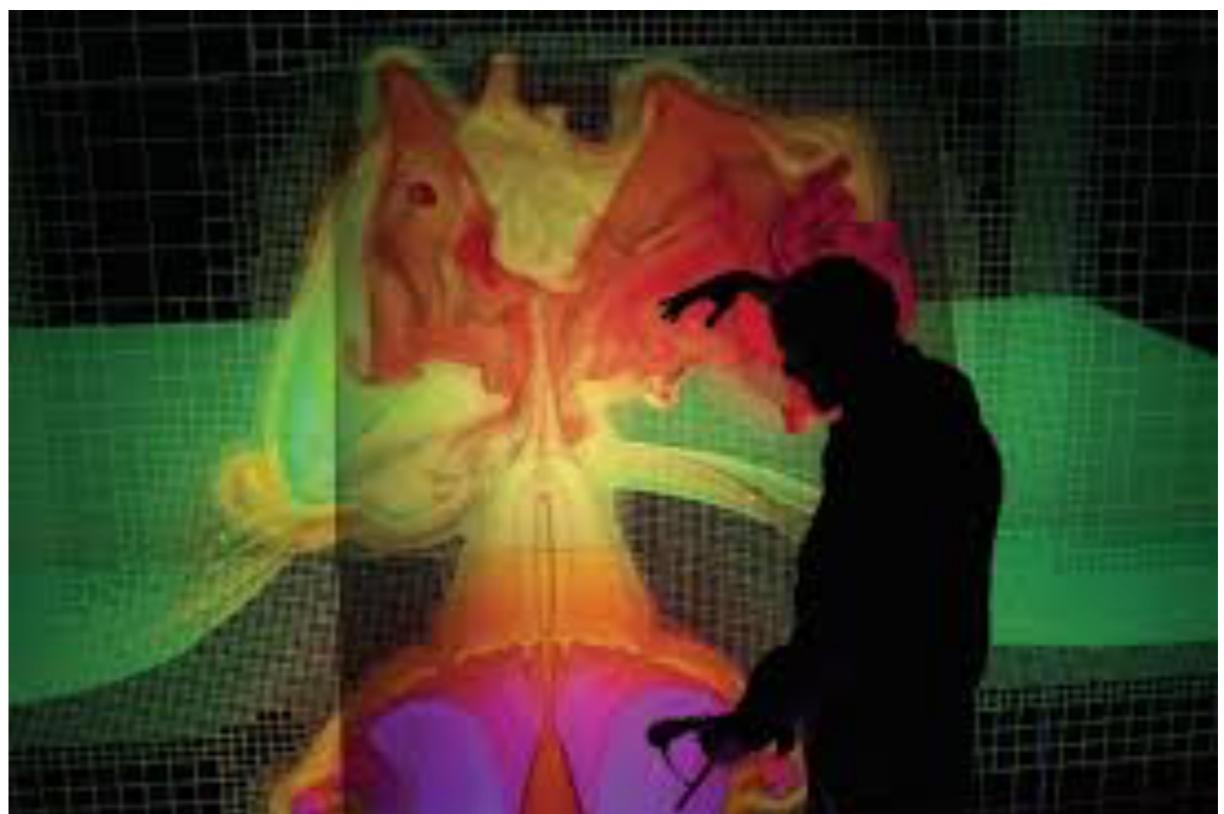
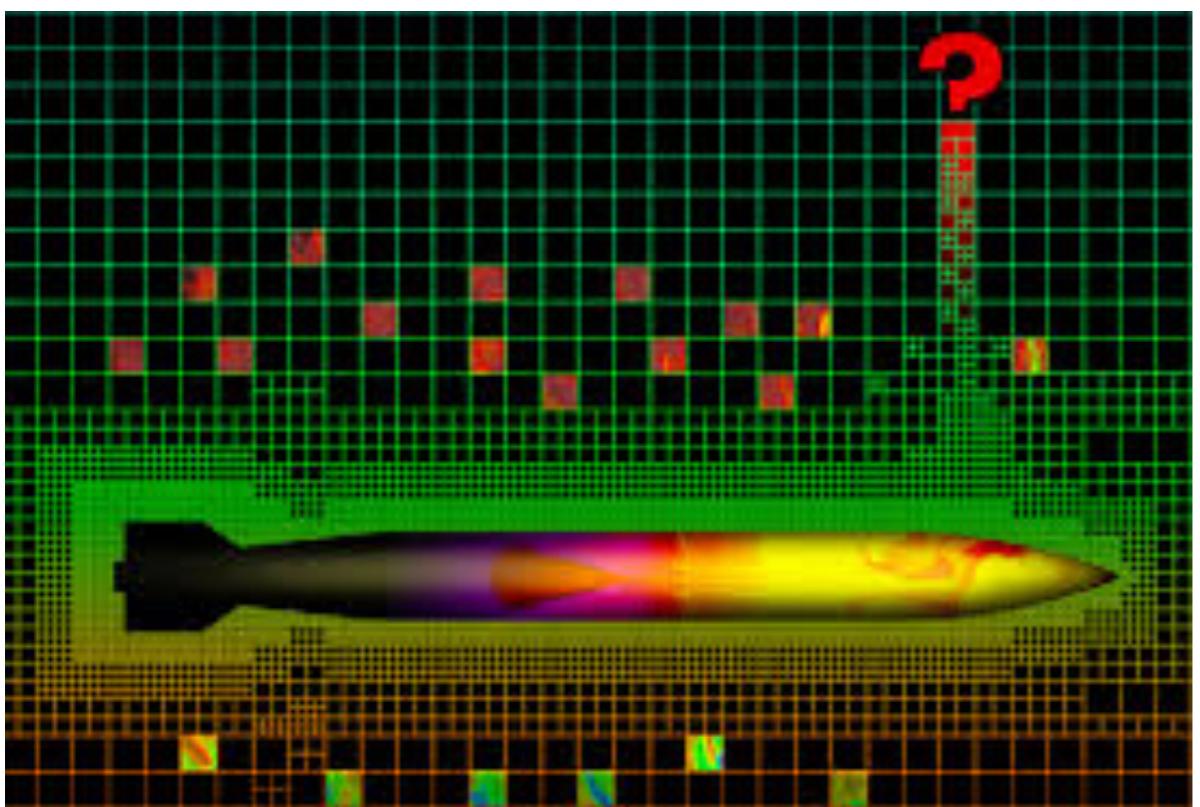
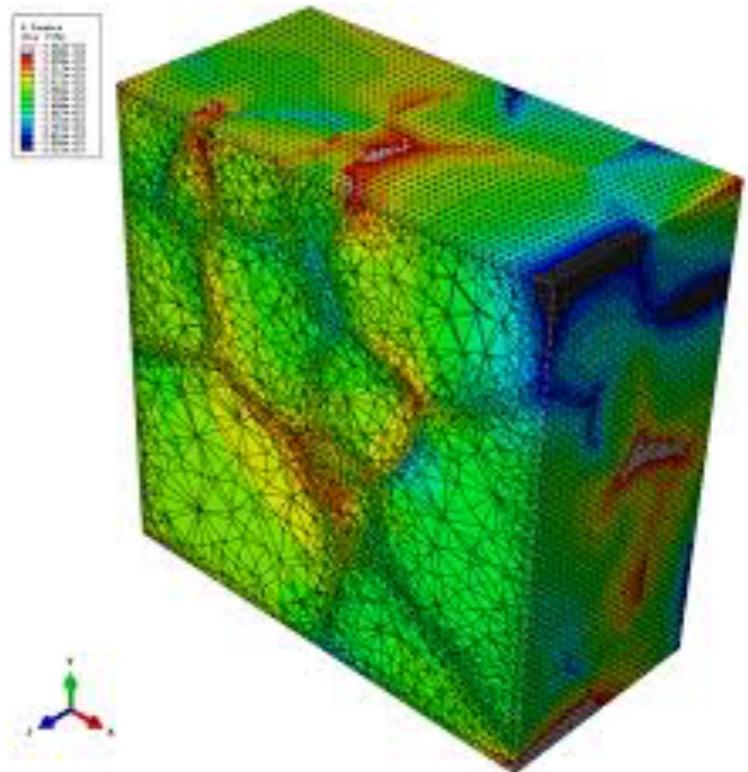
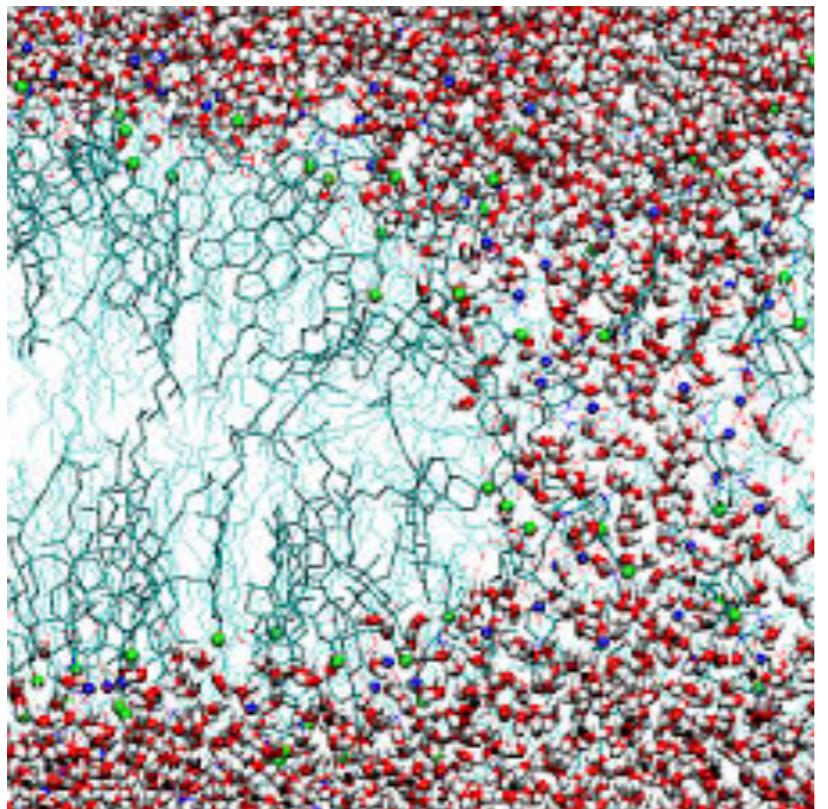
5.76 PFlops



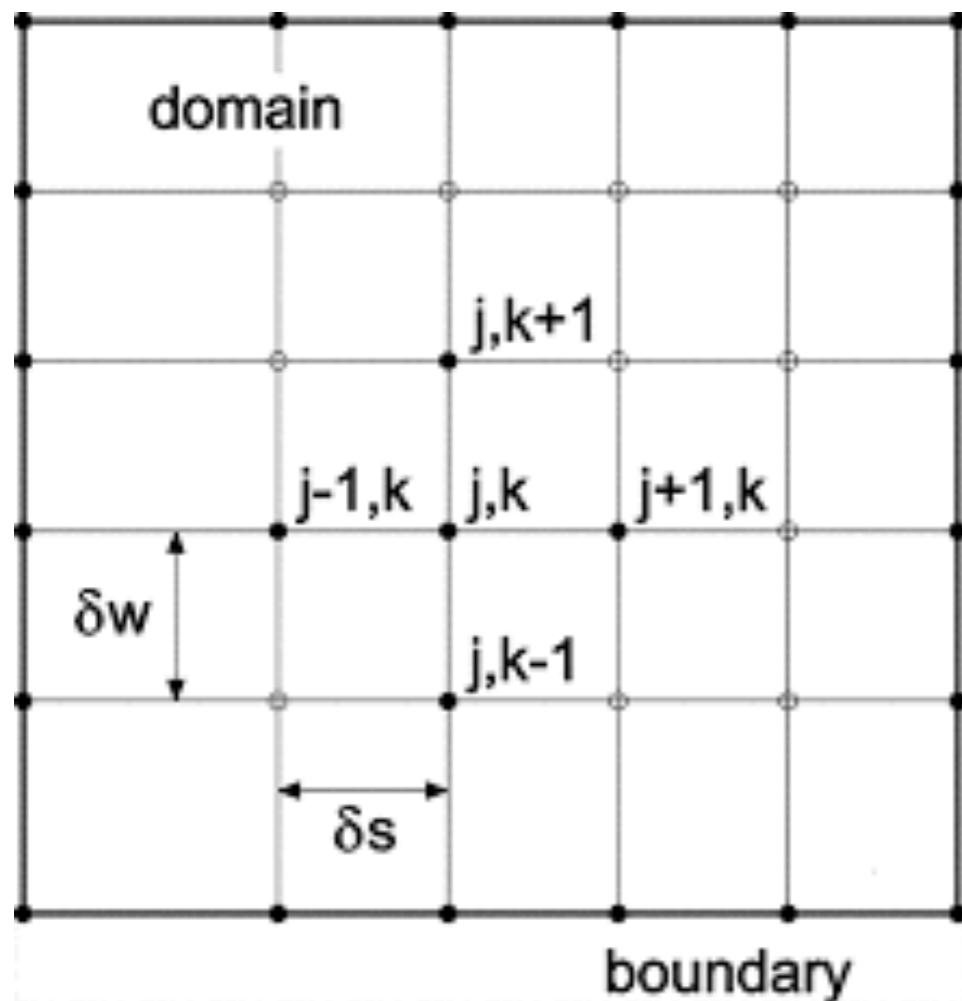
Simulation on TSUBAME



Discretization

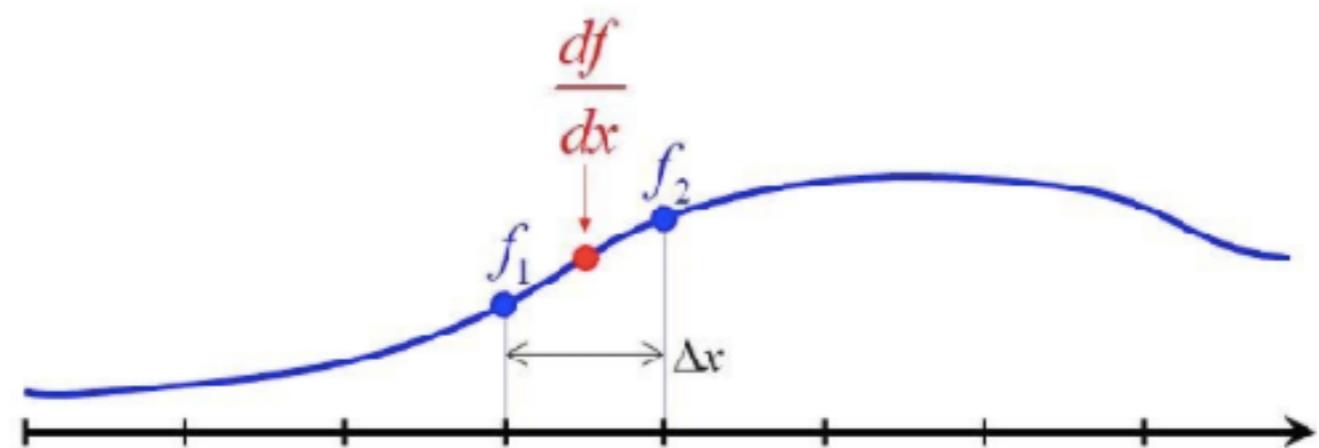


Finite difference methods



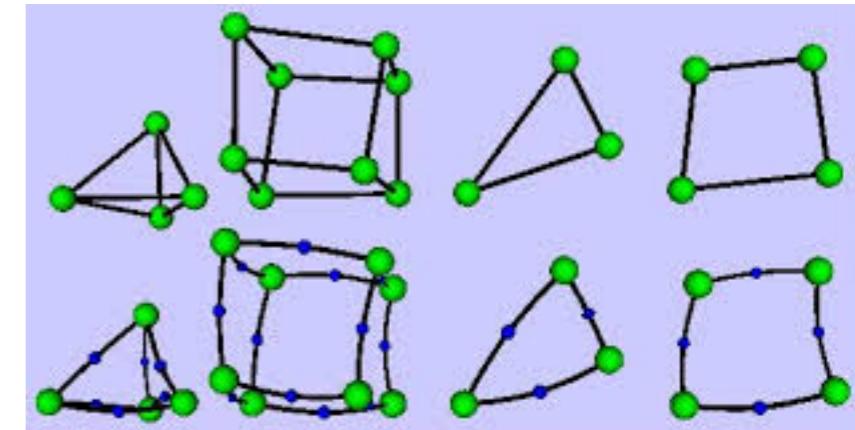
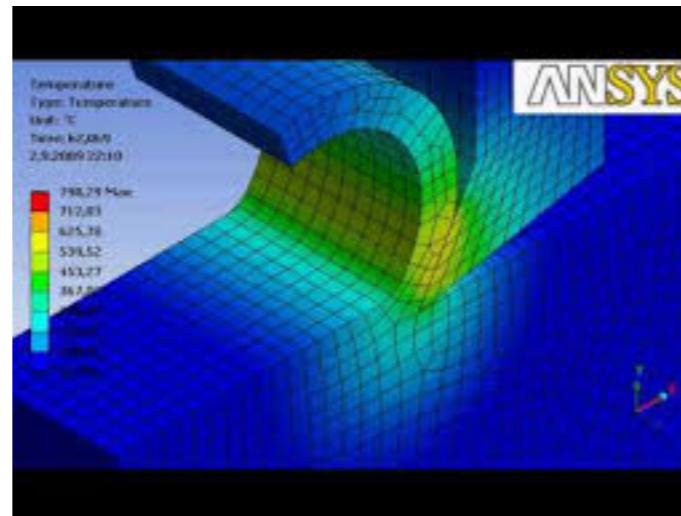
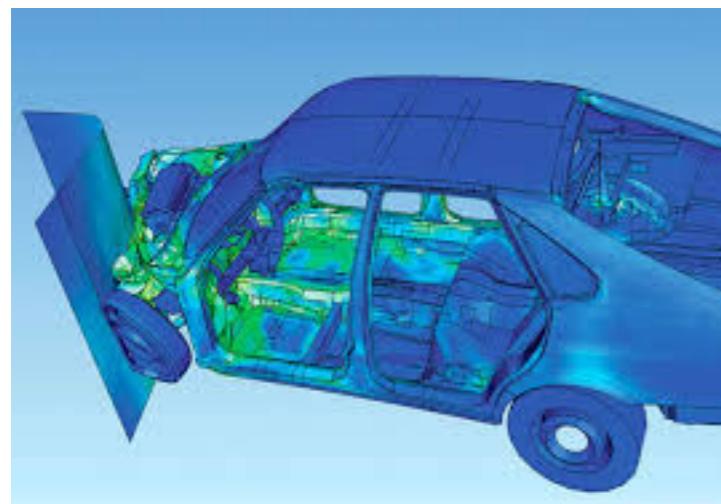
$$\frac{df_{1.5}}{dx} \approx \frac{f_2 - f_1}{\Delta x}$$

second-order accurate
first-order derivative

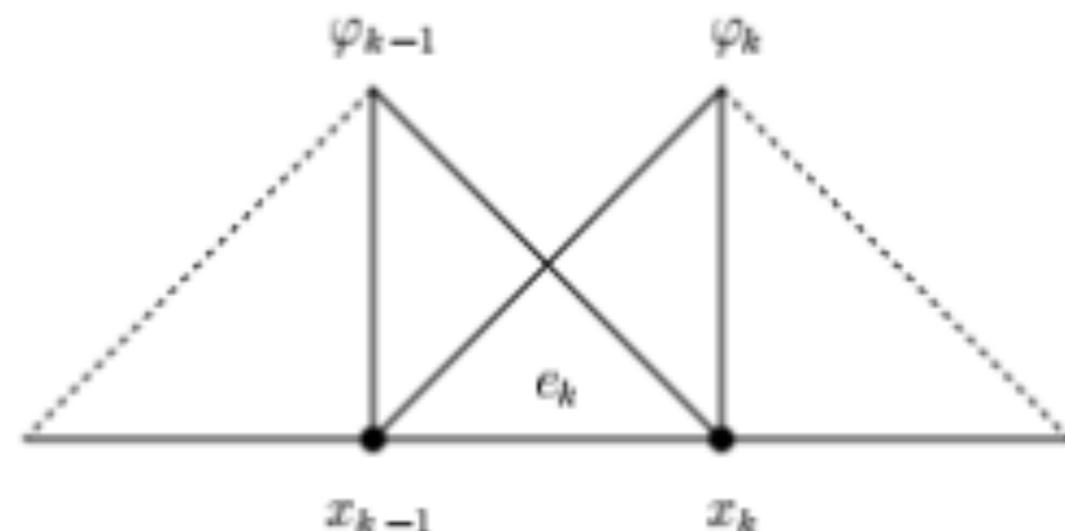


$$\frac{\partial p}{\partial t} + u \frac{\partial p}{\partial x} - D \frac{\partial^2 p}{\partial x^2} = 0$$

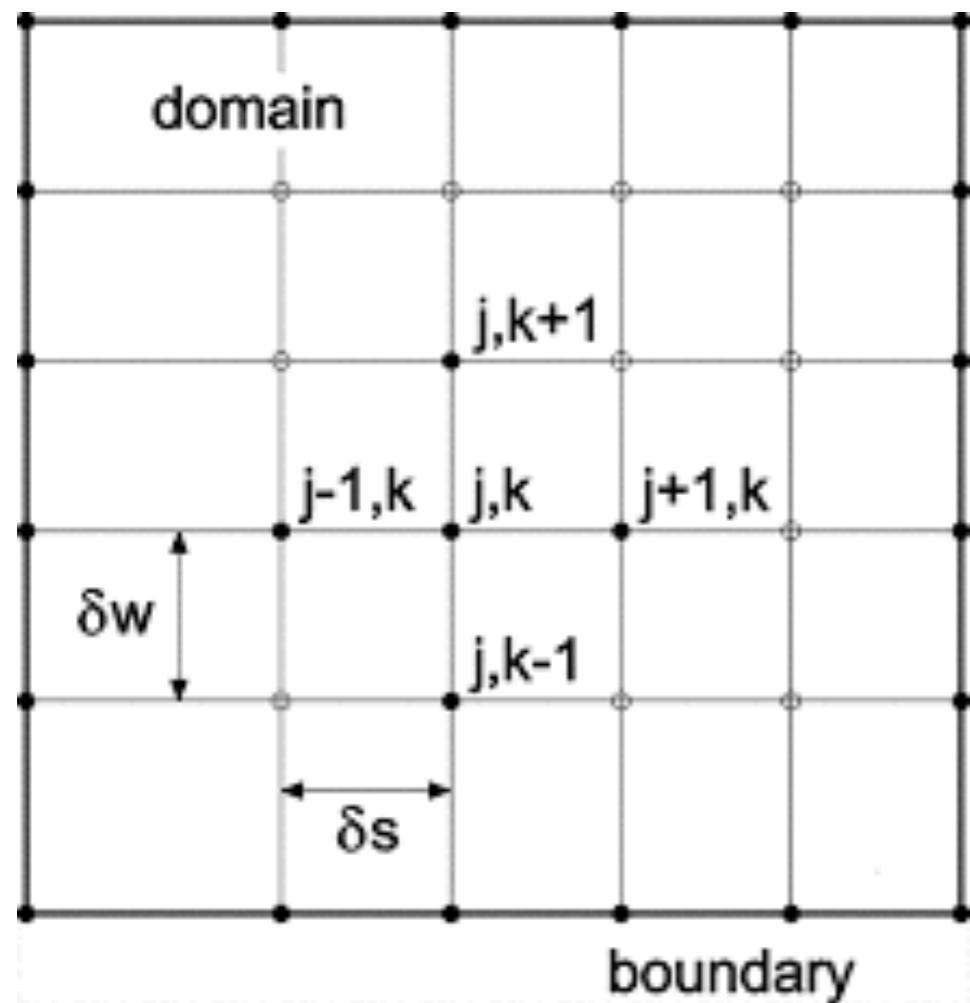
Finite element methods



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

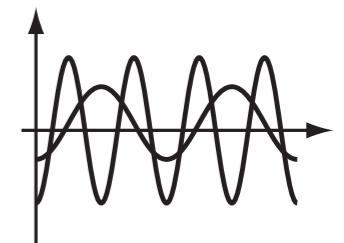


Spectral methods



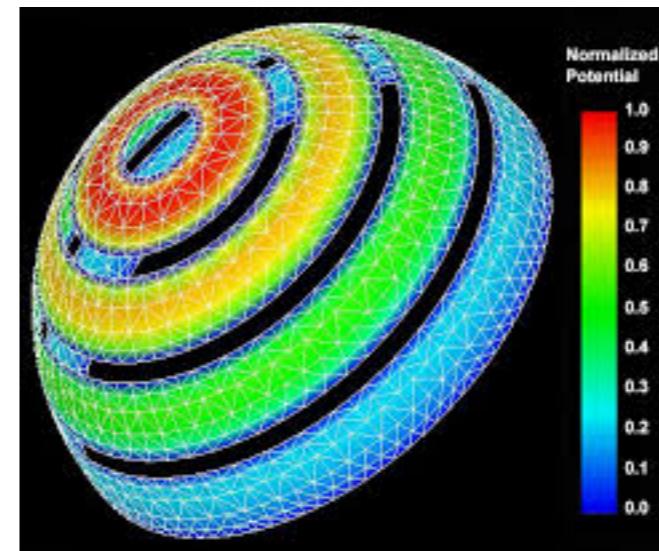
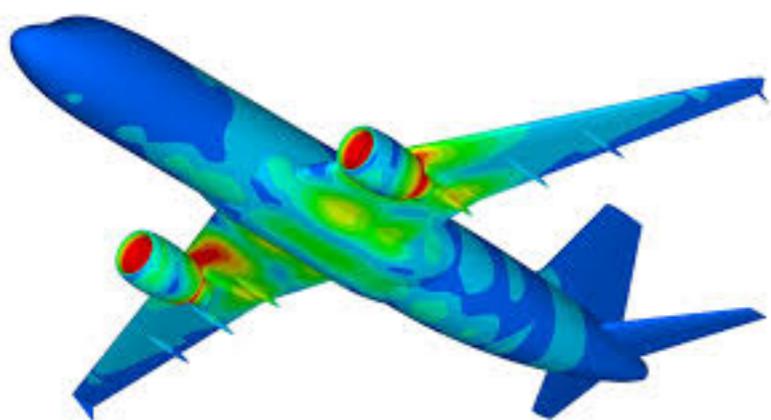
$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) f(x, y) = g(x, y)$$

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



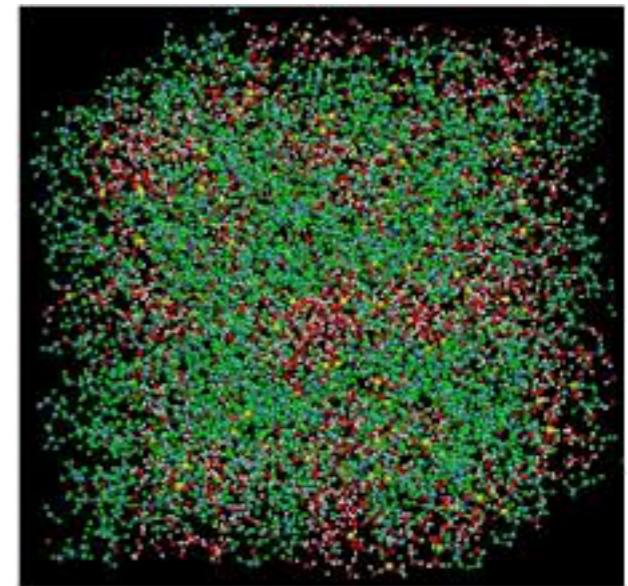
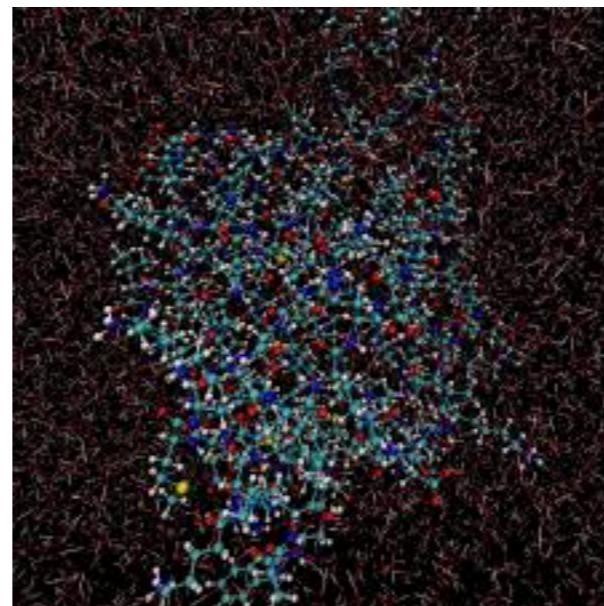
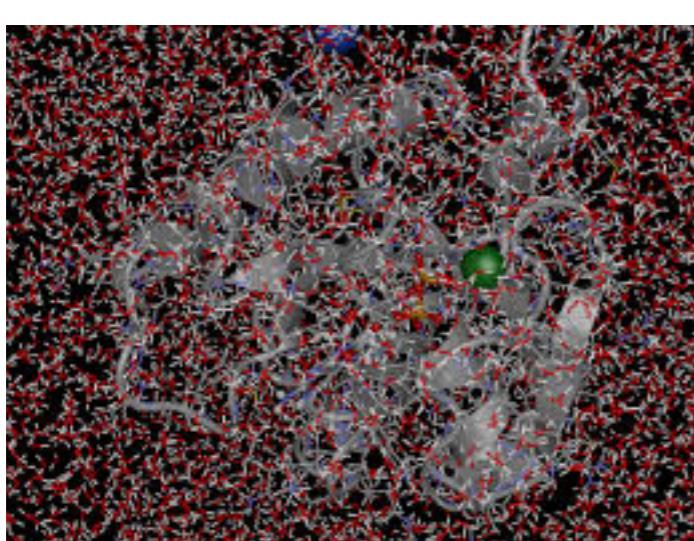
$$\sum -a_{j,k} (j^2 + k^2) e^{i(jx+ky)} = \sum b_{j,k} e^{i(jx+ky)}$$

Boundary element methods



$$\begin{aligned} & \int_{\Omega_b} \left(u^*(x, x_\theta) \nabla^2 u(x) - u(x) \nabla^2 u^*(x, x_\theta) \right) d\Omega \\ &= \int_{\Gamma_b} \left(u^*(x, x_\theta) \frac{\partial u(x)}{\partial n} - u(x) \frac{\partial u^*(x, x_\theta)}{\partial n} \right) d\Gamma_b(x) \end{aligned}$$

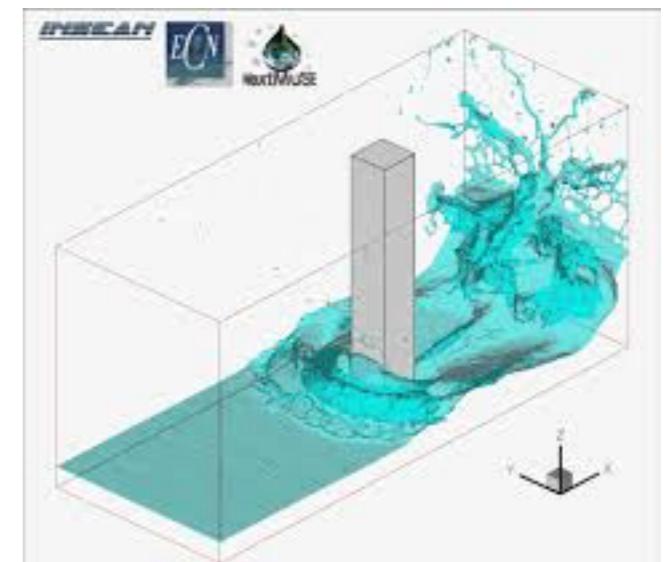
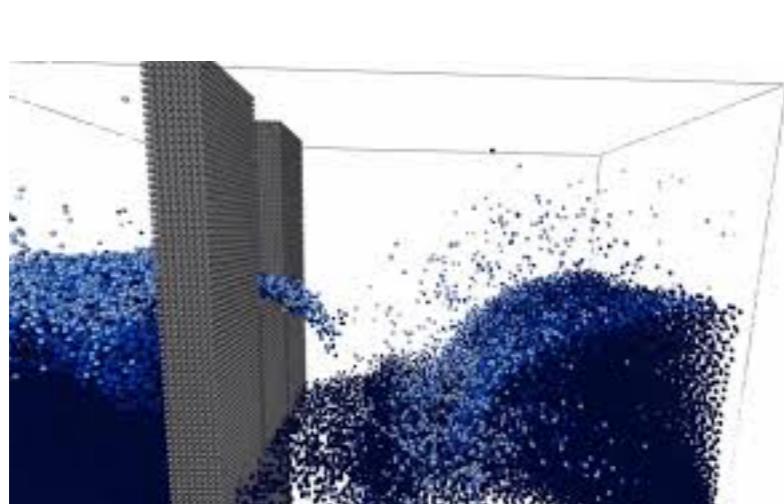
Molecular dynamics



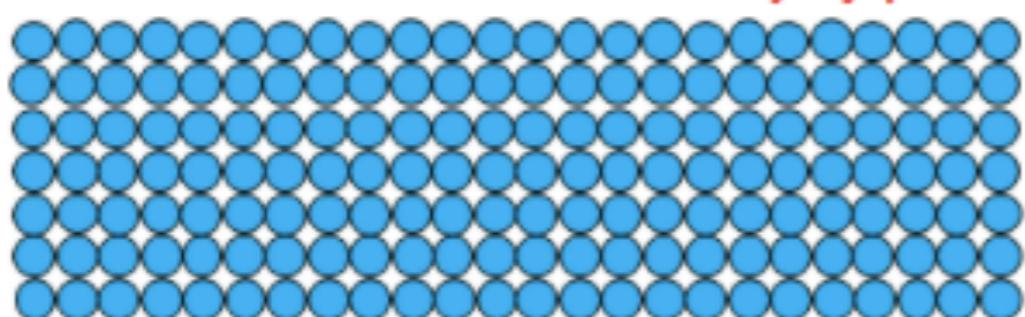
$$V = \sum_{bonds} \frac{1}{2} K_{ij}^b (r_{ij} - b_{ij})^2 + \sum_{angles} \frac{1}{2} K_{ijk}^{\theta} (\theta_{ijk} - \theta_{ijk}^0)^2 \\ + \sum_{dihedrals} K_{\varphi} (1 + \cos(n\varphi - \varphi_0)) \\ + \sum_{i \neq j} 4\epsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^6 \right] + \sum_{i \neq j} \frac{q_i q_j}{\epsilon_0 r_{ij}}$$

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

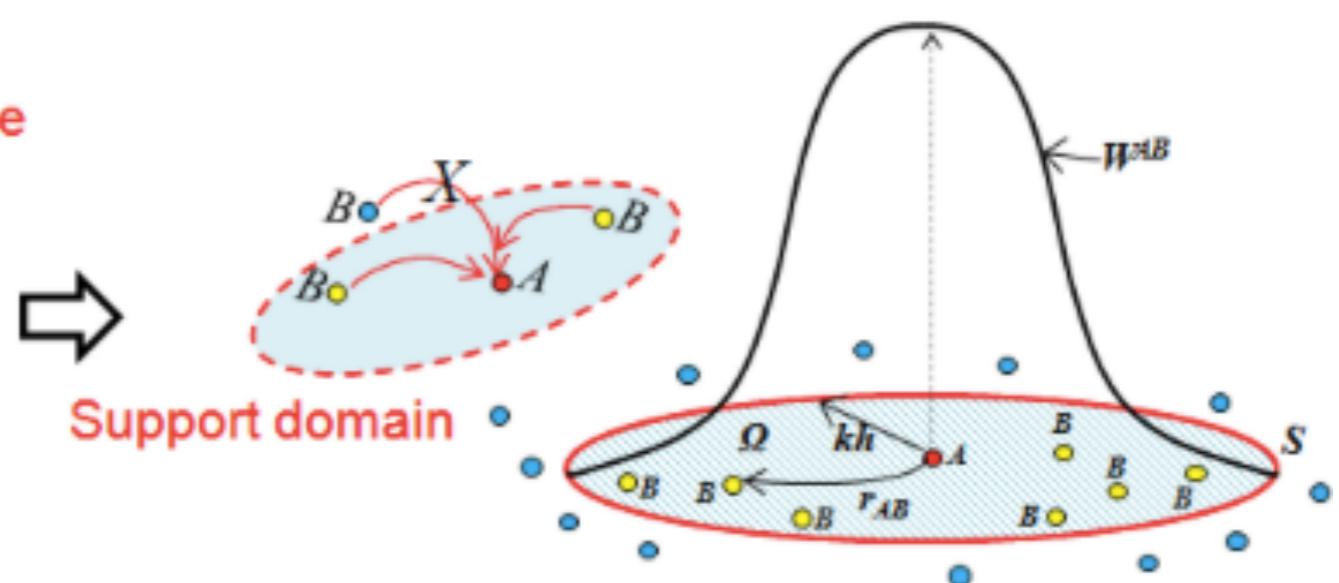
Smooth particle hydrodynamics



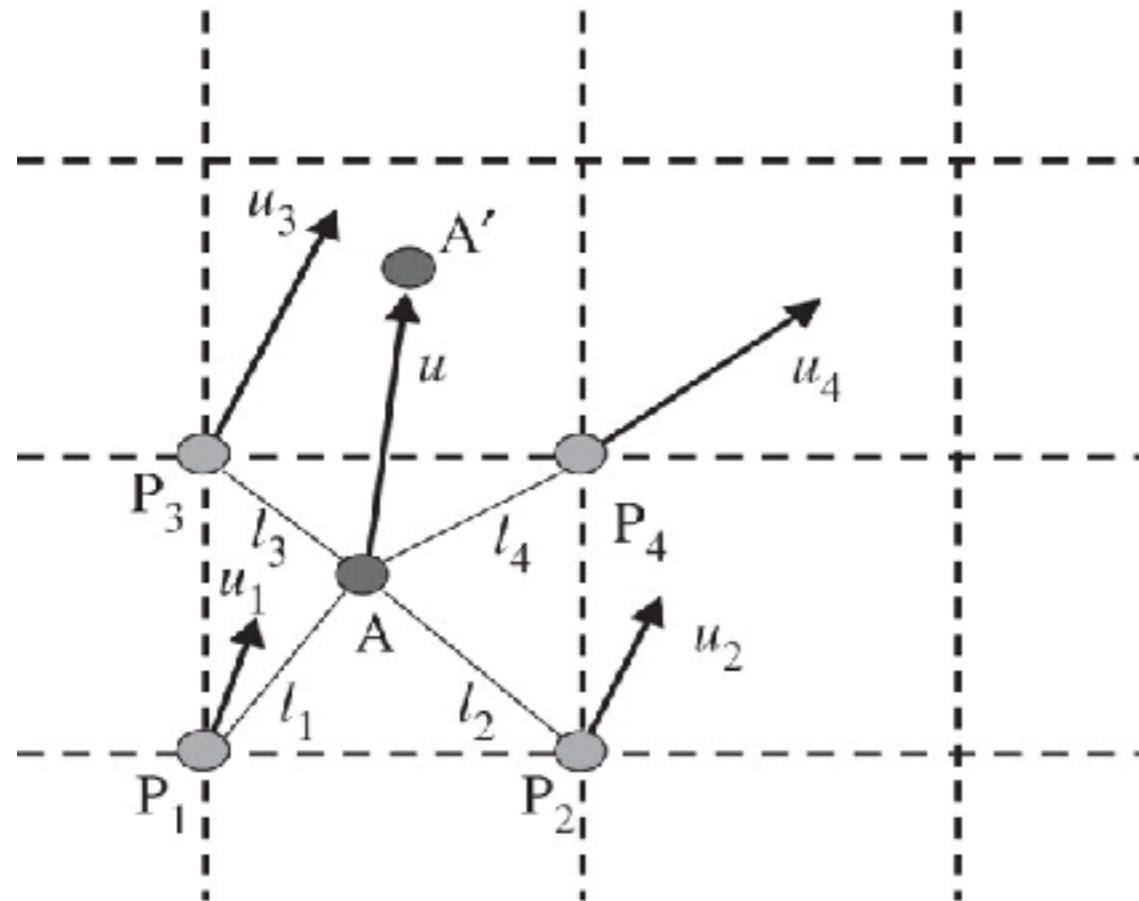
Discretization of continuum body by particle



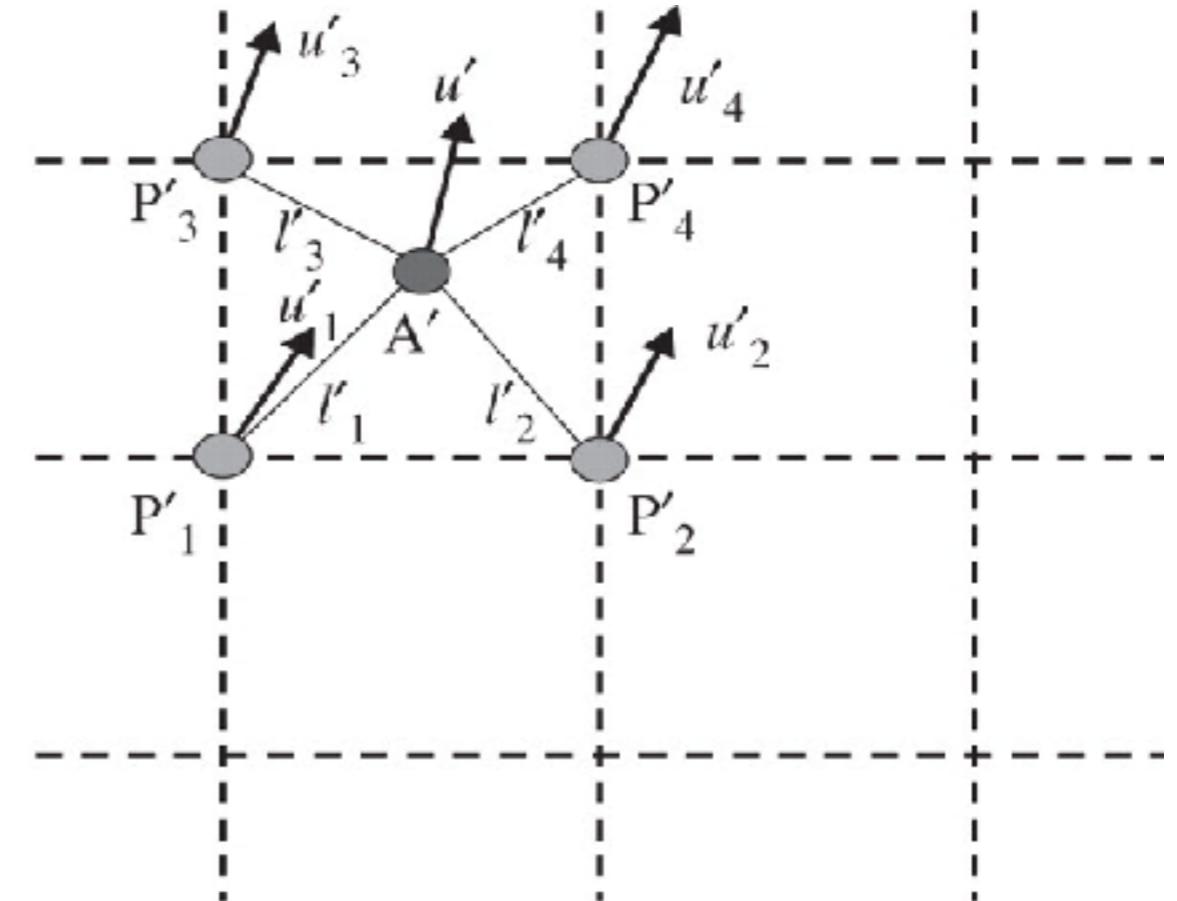
- Discretization Particle
- Target Particle A
- Neighbouring Particle B



Particle-mesh methods

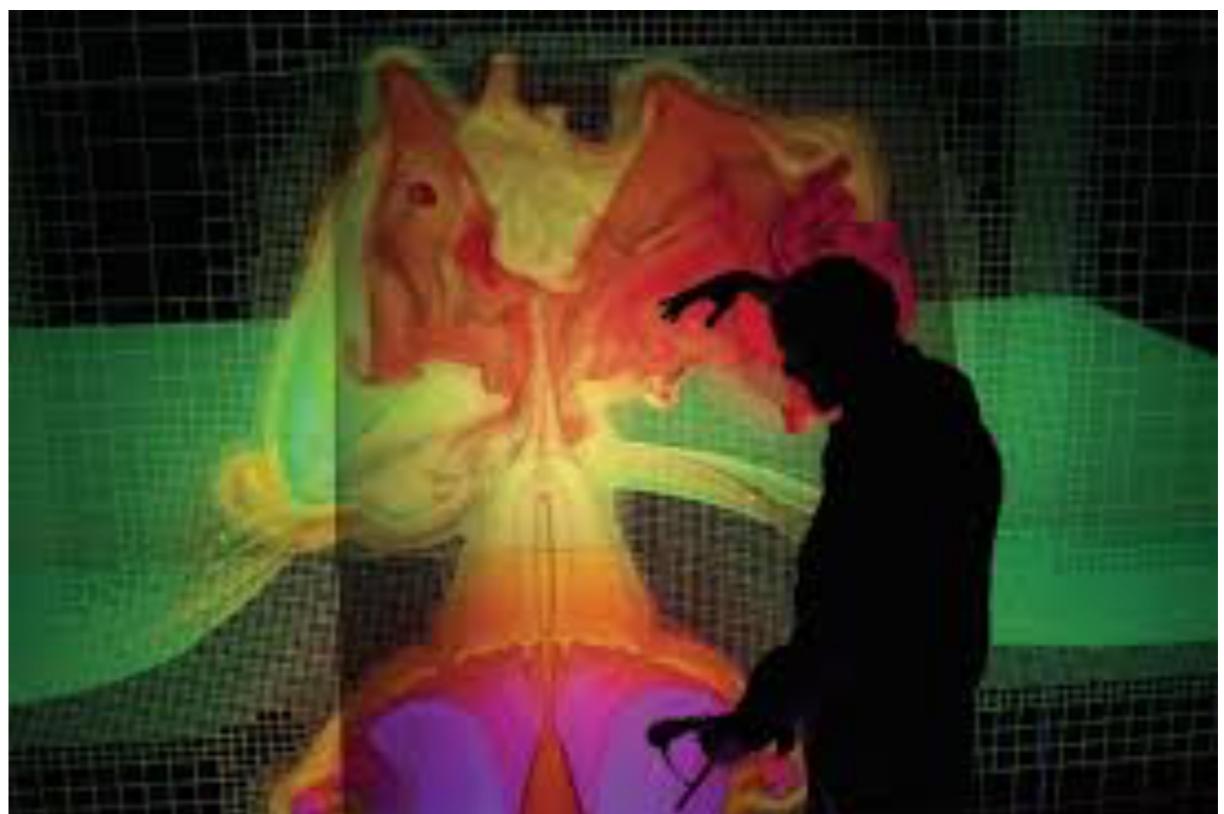
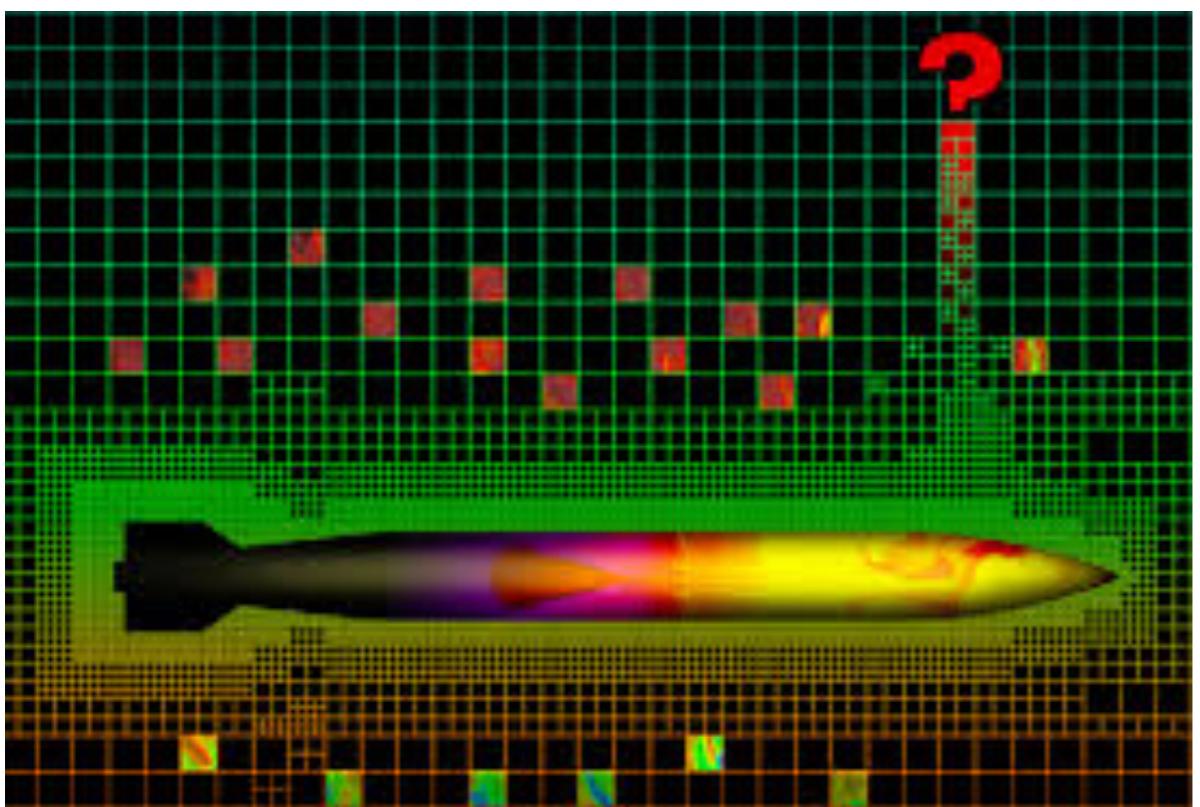
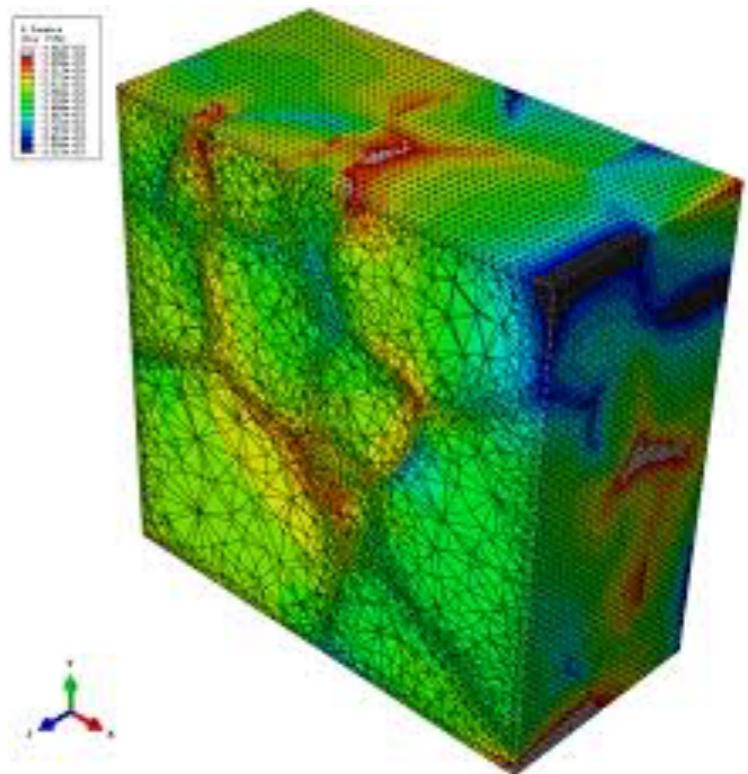
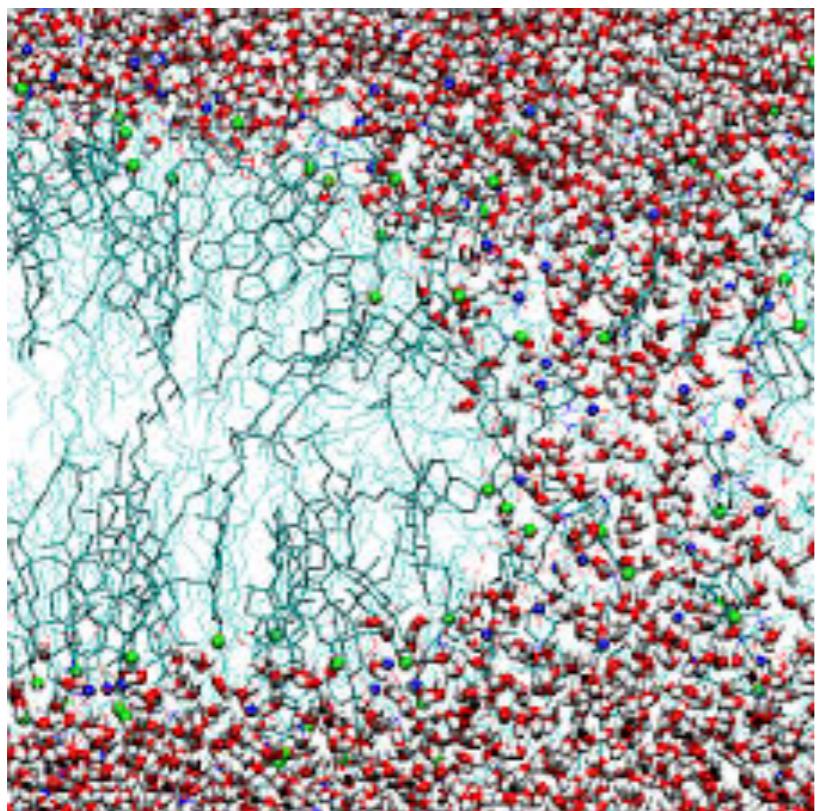


$$u = \frac{\frac{u_1}{l_1} + \frac{u_2}{l_2} + \frac{u_3}{l_3} + \frac{u_4}{l_4}}{\frac{1}{l_1} + \frac{1}{l_2} + \frac{1}{l_3} + \frac{1}{l_4}}$$

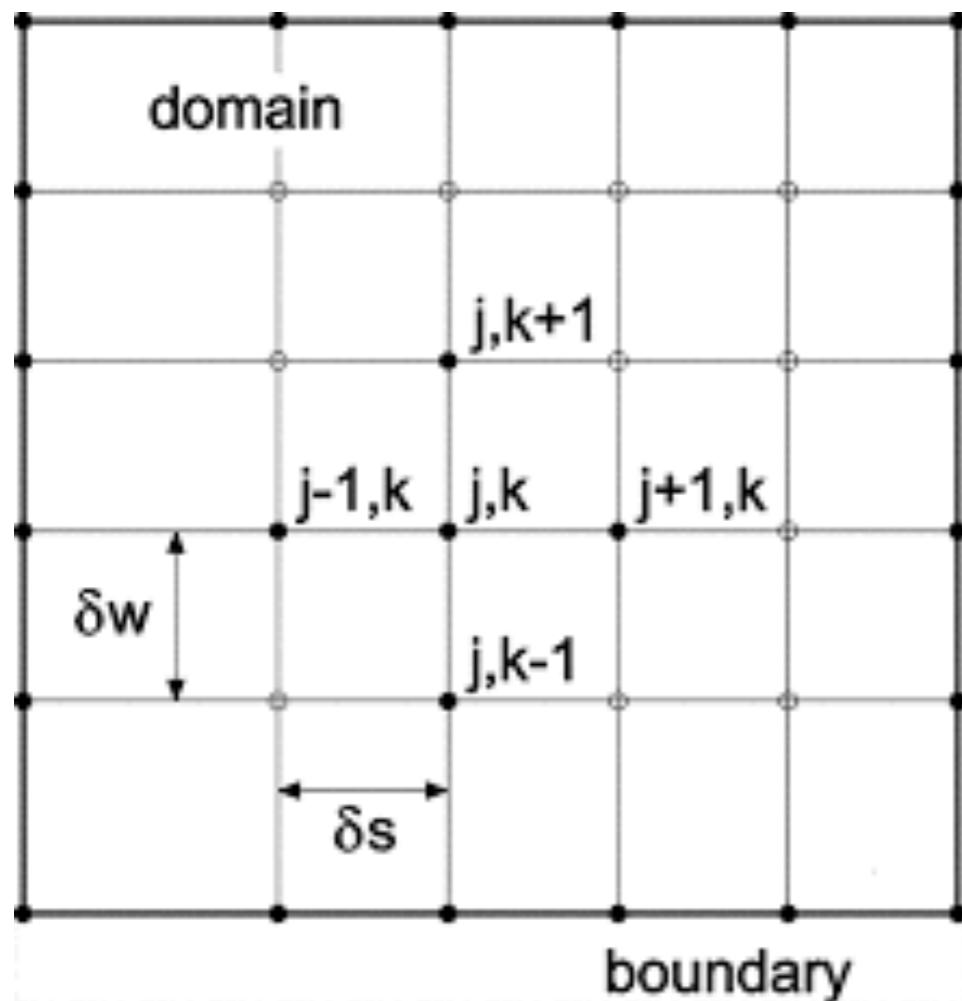


$$u' = \frac{\frac{u'_1}{l'_1} + \frac{u'_2}{l'_2} + \frac{u'_3}{l'_3} + \frac{u'_4}{l'_4}}{\frac{1}{l'_1} + \frac{1}{l'_2} + \frac{1}{l'_3} + \frac{1}{l'_4}}$$

Discretization

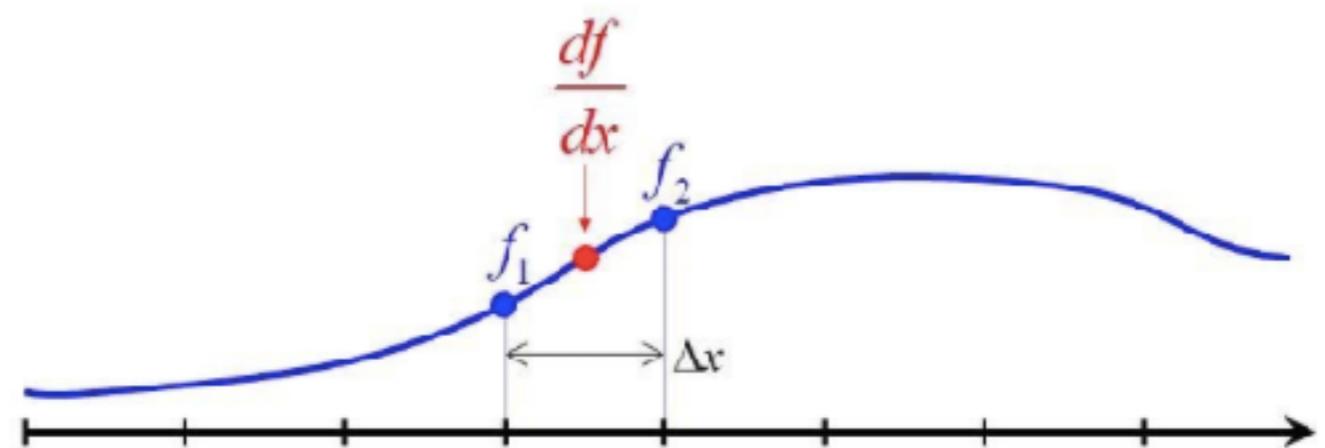


Finite difference methods



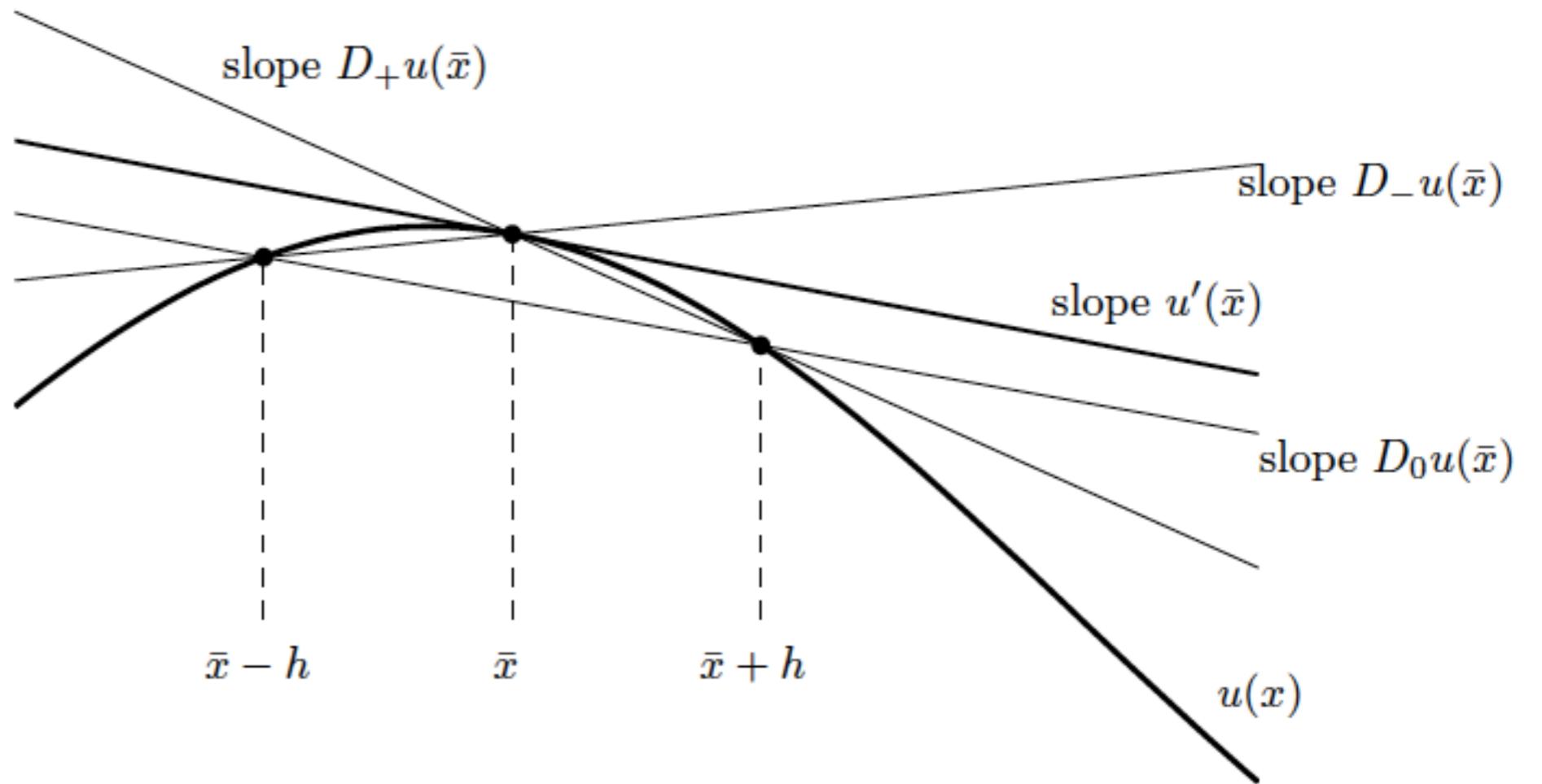
$$\frac{df_{1.5}}{dx} \approx \frac{f_2 - f_1}{\Delta x}$$

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

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

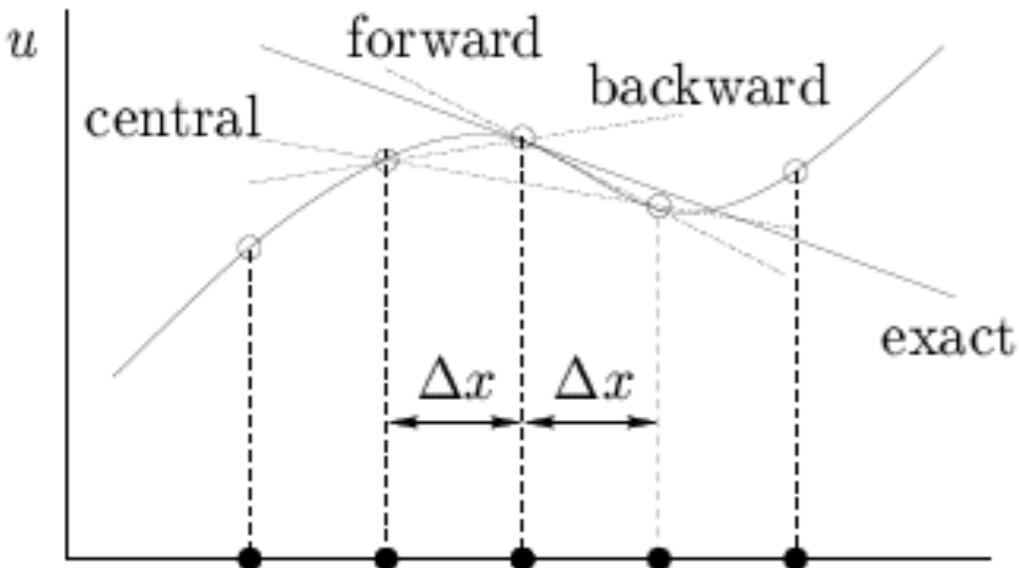
Backward difference

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

Central difference

$$D_0 u(\bar{x}) \equiv \frac{u(\bar{x} + h) - u(\bar{x} - h)}{2h} = \frac{1}{2}(D_+ u(\bar{x}) + D_- u(\bar{x}))$$

Truncation error



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

forward difference

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

backward difference

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

central difference

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

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

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

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

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

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

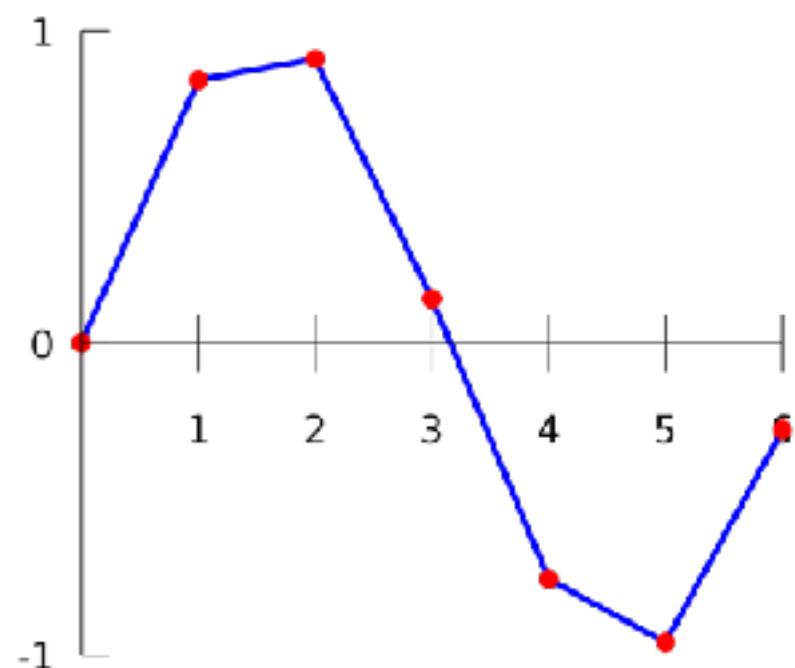
$$\frac{f(x+h) - 2f(x) + f(x-h)}{h^2} = f''(x) + e^h(x)$$

Alternatively, we can use forward and backward approximations:

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

or the other way around

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



	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.