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I.C.T.P., P.O. BOX 586, 34100 TRIESTE, ITALY, CABLE: CENTRATOM TRIESTE

WINTER COLLEGE ON "MULTILEVEL TECHNIQUES IN COMPUTATIONAL PHYSICS"

Physics and Computations with Multiple Scales of Lengths
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Coarsening Particle Calculations

A. Brandt
The Weizmann Institute of Sciences
Rehovot. Israel

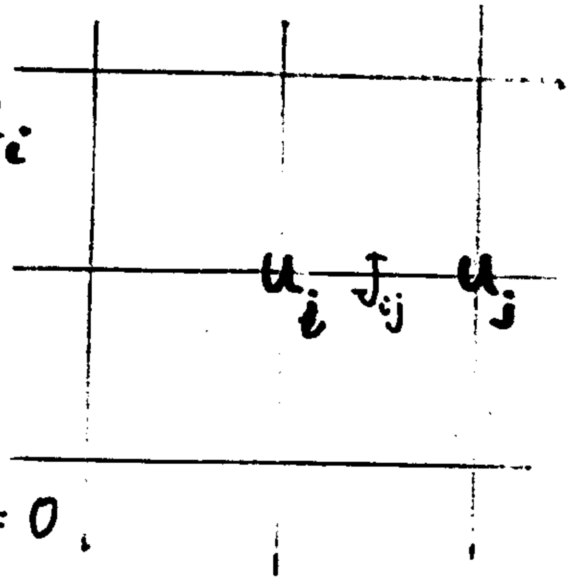
Grids ⟷ Particles

Long range interactions	✓	✓
Local optimization	✓	•
Global optimization	Th	Th
Monte Carlo simulations	✓W	•
Dynamics	✓	
Macroscopic equations	✗W	•

$$-\Delta u = f \quad \Longleftrightarrow$$

$$E(u) = \int \left[\left(u_x^2 + u_y^2\right)/2 - fu \right] dx\,dy = \min!$$

$$E^h(u) = \frac{1}{2} \sum_{\langle i,j \rangle} \left(\frac{u_i - u_j}{h} \right)^2 - \sum_i f_i u_i$$



$$E^h(u) = \min!$$

$$\Longleftrightarrow \quad \frac{\partial E^h}{\partial u_i} = \frac{1}{h^2} \sum_{\langle i,j \rangle} (u_i - u_j) - f_i = 0 .$$

$$-\nabla (J \nabla u) = f \quad \Longleftrightarrow$$

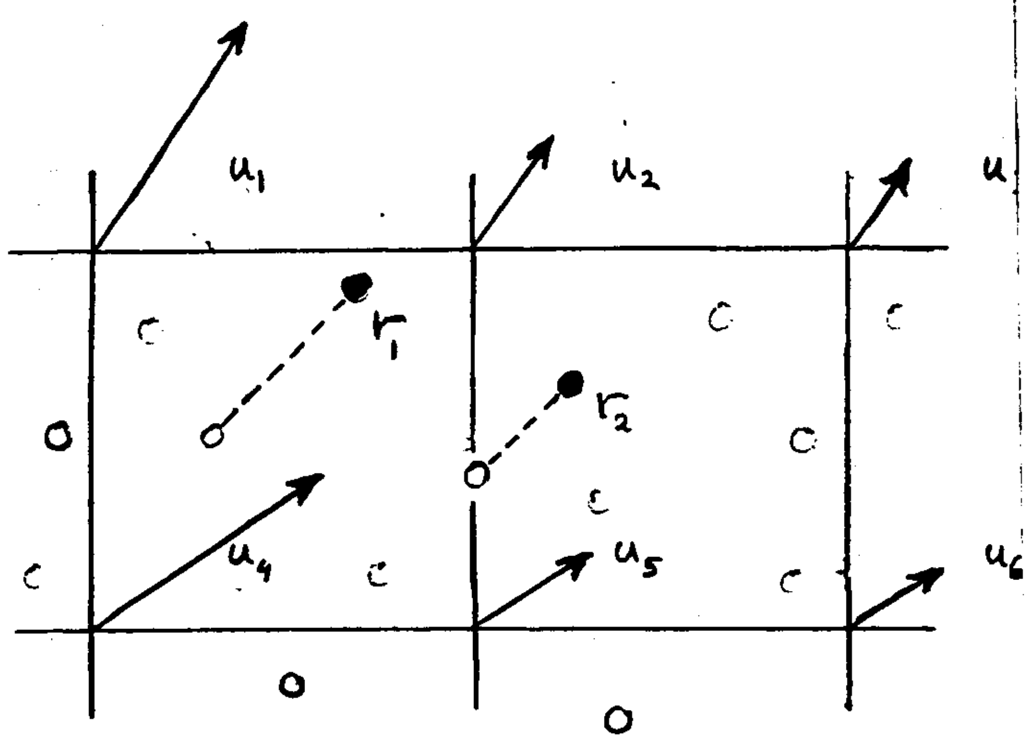
$$E(u) = \frac{1}{2} \int \left[(J u_x)^2 + (J u_y)^2 - fu \right] dx\,dy$$

$$E^h(u) = \frac{1}{2h^2} \sum_{\langle i,j \rangle} J_{ij} \left(u_i - u_j \right)^2 - \sum_i f_i u_i$$

$$= -\frac{1}{h^2} \sum_{\langle i,j \rangle} J_{ij}\, u_i\, u_j - \sum_i f_i u_i$$

$$+ \frac{1}{2h^2} \sum_{\langle i,j \rangle} J_{ij} \left(u_i^2 + u_j^2 \right)$$

displacement field:



$$r_1 = r_1^\circ + \sum \lambda_{1j} u_j \,, \qquad \sum_j \lambda_{1j} = 1$$

$$r_1 - r_2 = r_1^\circ - r_2^\circ + \sum \left(\lambda_{1j} - \lambda_{2j}\right) u_j$$

$$= A + \sum B_{ij} \left(u_i - u_j\right)$$

$$E = \sum_{\alpha,\beta} V\left(|r_\alpha - r_\beta|\right)$$

$$\approx \alpha + \sum_{i,j} \beta_{ij} \left(u_i - u_j\right) + \sum_{i,j} \gamma_{ij} \left(u_i - u_j\right)^2 + \cdots$$

$$|u_i - u_j| < \mu_{ij}$$

Elasticity, **plasticity**, strain limits

$$r^h = (r_1, r_2, \ldots) = r^{h0} + I_H^h u^H$$

$$E(r^h) = E\left(r^{h0} + I_H^h u^H\right)$$
$$\equiv E^H(u^H)$$

$AU = b$ on grid h, A symm. pos. def.

$$\frac{1}{2} U^T A U - U^T b = \min!$$

$I_{2h}^h V^{2h}$ coarse-grid correction to u: $U \approx u + I_{2h}^h V^{2h}$

$\Downarrow$

minimize

$$\frac{1}{2}\left(u + I_{2h}^h V^{2h}\right)^T A \left(u + I_{2h}^h V^{2h}\right) - \left(u + I_{2h}^h V^{2h}\right)^T b$$

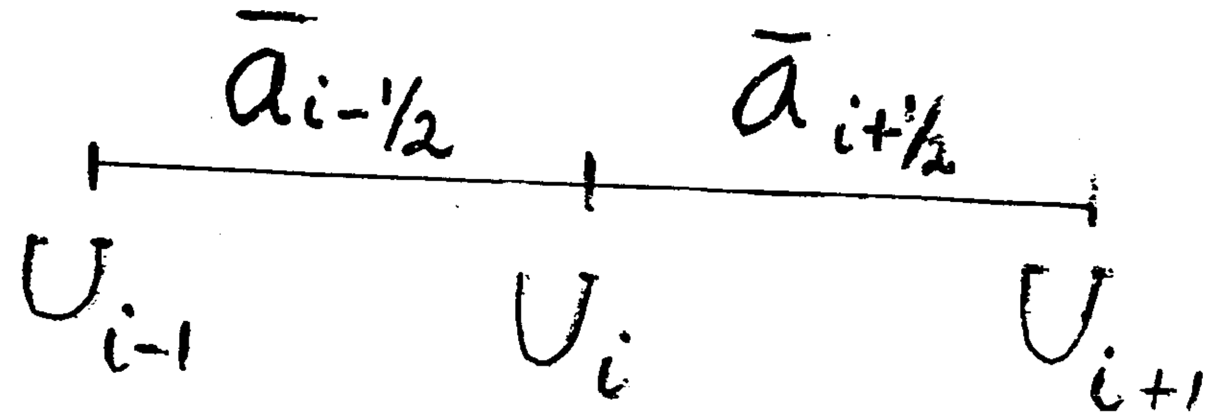
$$\frac{1}{2} V^{2hT} \underline{I_{2h}^{hT} A I_{2h}^h} V^{2h} - V^{2hT} \underline{I_{2h}^{hT}(b - Au)}$$

$A^{2h} V^{2h} = R^{2h}$ where

$$A^{2h} = I_{2h}^{h\,T} A I_{2h}^h, \quad R^{2h} = I_{2h}^{h\,T}(b - Au)$$

, Symmetric, Conservative   Full Weighting

$$(aU_x)_x + (bU_y)_y = F$$



$$\frac{\bar{a}_{i+1/2}(U_{i+1}-U_i)-\bar{a}_{i-\frac{1}{2}}(U_i-U_{i-1})}{h^2}$$

Symmetric matrix.

Conservation form better approximat (flux is smoother)

$$Lu \equiv (au_x)_x + (bu_y)_y = f(x,y,u)$$

Alcouffe Brandt Dendy Painter

$\varepsilon < a(x,y,u),\ b(x,y,u) < \frac{1}{\varepsilon}$ discontinuously

Interpolation: Based on relaxed error V. $LV \approx 0$

Linear interpolation when u_x continuous

but here: continuity of the flux $\cancel{au_x}$ aV_x

$$I_{2h}^h V^{2h}{}_i = \frac{\bar{a}_{i-1/2} V^{2h}_{i-1} + \bar{a}_{i+1/2} V^{2h}_{i+1}}{\bar{a}_{i-1/2} + \bar{a}_{i+1/2}}$$

$\bar{a}$ proper average

Coarse-grid problem: $\left(I_h^{2h} L^h I_{2h}^h\right) V^{2h} = I_h^{2h} R^h$, $\quad I_h^{2h} = I_{2h}^{h\,T}$

$$\Leftrightarrow \quad \min\ \mathcal{F}\left(u^h + I_{2h}^h V^{2h}\right), \qquad \mathcal{F}(w^h) = \left(L^h w^h, w^h\right) - 2\left(f^h, w^h\right)$$

$\Downarrow$

Black-Box MG: for any symmetric 9-point L^h.

Den[dy]

Algebraic MG (AMG): for general positive-type symmetric

Brandt McCormick Ruge

Systems: e.g.

$$L^h p_n - \alpha (p_n - p_w) = f$$
$$L^h p_w - \alpha (p_w - p_n) = g$$

n particles

$$E = \sum_{\alpha,\beta} V(|r_\alpha - r_\beta|)$$

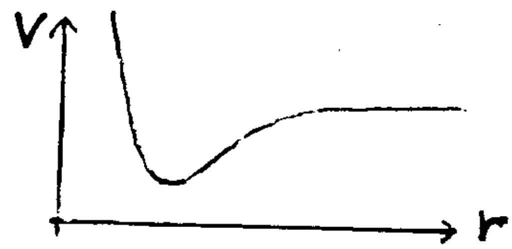
Long range forces

$V = a/r$: electrostatic, gravity, vortices ...

- $O(n)$ calculation of forces

  Coarse level: density

Short range forces



$V = a/r^{12} - b/r^{6}$: atomic

- fast local convergence

  Coarse level: Elasticity, plasticity

  strain limits with "breaks"

- Global minimization

  Multi-level stochastic optimization

Long + Short

charge density + elastic displacement field

Chains

"pressure"