An implementation of the Fast Multipole Method without multipoles

Robin Schoemaker

Scientific Computing Group Seminar

The Fast Multipole Method – Theory and Applications

Spring 2002

Overview

- Fast Multipole Algorithm
- Anderson’s method
  - Poisson’s formula instead of multipole expansions
- Application

N-body interactions (1)

- Particle simulations in physical systems require the evaluation of a potential function $\phi(\mathbf{r})$, (yielding a force field);
- These pair wise interactions are Coulombic/gravitational in nature:

$$\phi\left(\mathbf{r}_j\right) = \sum_{i=1}^{N} q_i \log\left|\mathbf{r}_j - \mathbf{r}_i\right| \ , \quad j = 1, \ldots, N$$

for a system of N charged particles in **2** dimensions with strengths q_i .

N-body interactions (2)

If N is the total number of particles involved, the temporal complexity of such a system is $O\left(N^2\right)$.

Multipole expansion

For m charges of strengths $\{q_i, i = 1,\ldots,m\}$ located at points $\{z_i, i = 1,\ldots,m\}$, with $|z_i| < r$, the potential $\phi(z)$ is approximated by the multipole expansion

$$\phi(z) \doteq \log(z)\sum_{i=1}^{m} q_i + \sum_{k=1}^{p} \frac{a_k}{z^k} \quad \text{with} \quad a_k = \sum_{i=1}^{m} \frac{-q_i z_i^k}{k},$$

for any $z \in \mathbb{C}$ with $|z| > r$.

Error bound

For $A = \sum_{i=1}^{m} \left| q_i \right|$ and any $p \geq 1$,

$$\left| \phi(z) - \log(z) \sum_{i=1}^{m} q_i - \sum_{k=1}^{p} \frac{a_k}{z^k} \right| \leq \left(\frac{A}{|z/r| - 1} \right) \left(\frac{1}{|z/r|} \right)^p$$

$$\leq A \left(\frac{1}{2} \right)^p \text{, for } |z/r| \geq 2.$$

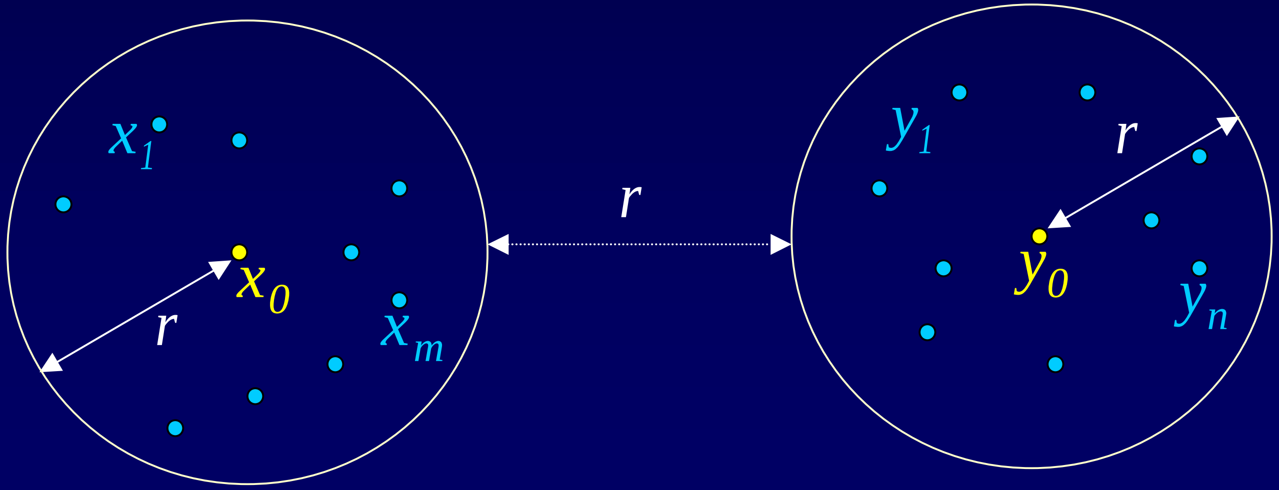
Example of speed-up (1)

Two sets of charges are well-separated :

$$|x_i - x_0| < r \quad \text{for} \ \ i = 1, \ldots, m \ ,$$

$$|y_j - y_0| < r \quad \text{for} \ \ j = 1, \ldots, n \ ,$$

$$|x_0 - y_0| > 3r \ .$$

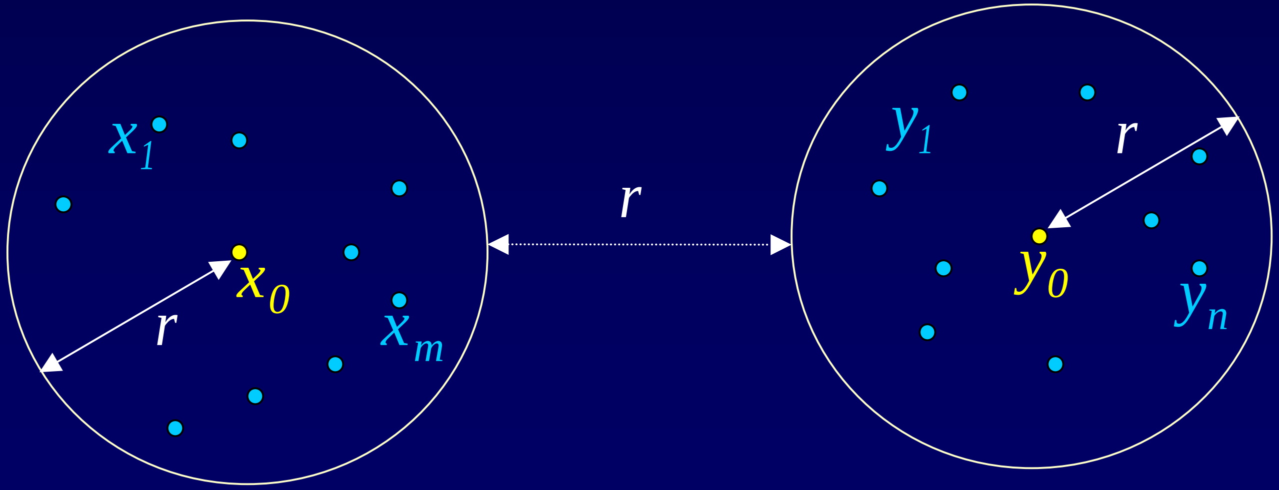


Example of speed-up (2)

The potential at the points $\{y_i\}$ due to charges at $\{x_j\}$ is computed directly via

$$\sum_{i=1}^{m} \phi_{x_i}\left(y_j\right) \quad \text{for all} \quad j = 1, \ldots, n \quad \text{and requires}$$

$O(nm)$ computations (evaluating m fields at n points).



Example of speed-up (3)

- A p-term multipole expansion due to charges $q_1, \ldots, q_m$ about x_0 requires $O(mp)$ operations;
- Evaluating this expansion at all $\{y_i\}$: $O(np)$ operations; total : $O(mp + np)$

The $O(p)$ operations can be neglected
for large m and n, resulting in
$O(m) + O(n) << O(mn)$.

Translation operators

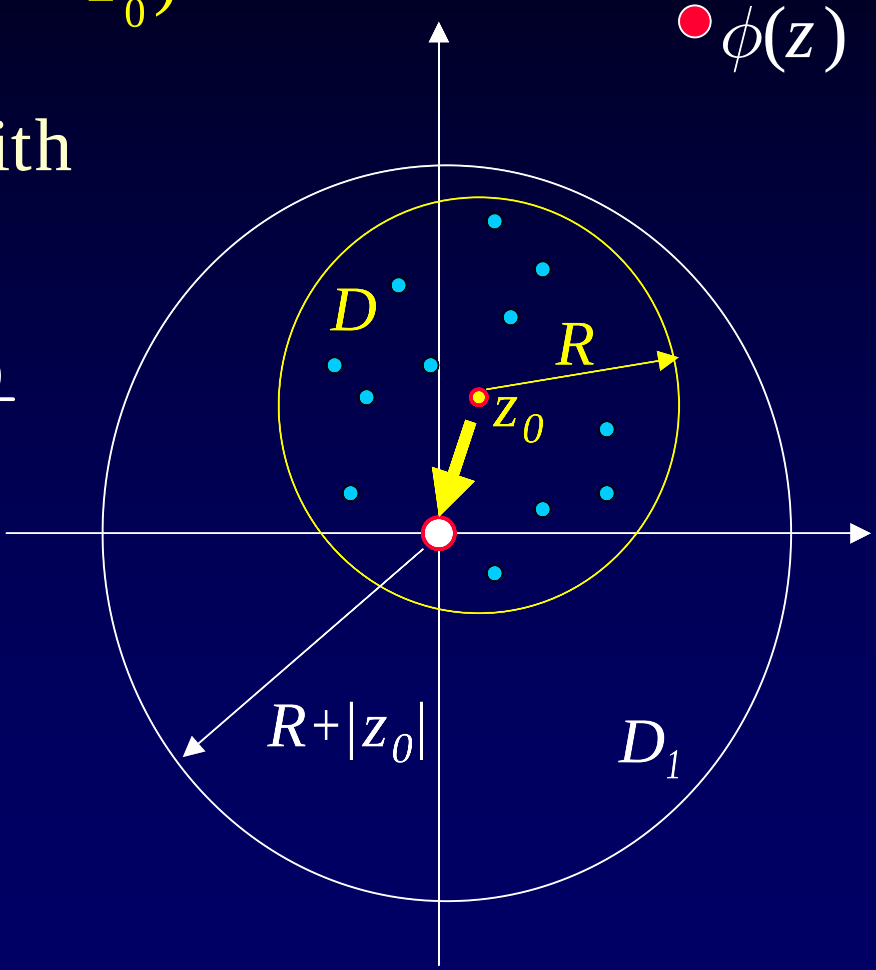
- Shifting the centre of a multipole expansion: M2M;
- Convert a shifted expansion into a local (Taylor) expansion: M2L;
- Shifting the centre of a local (Taylor) expansion: L2L.

M2M

$$\phi(z) \doteq a_0 \log(z - z_0) + \sum_{k=1}^{p} \frac{a_k}{(z - z_0)^k}$$ into

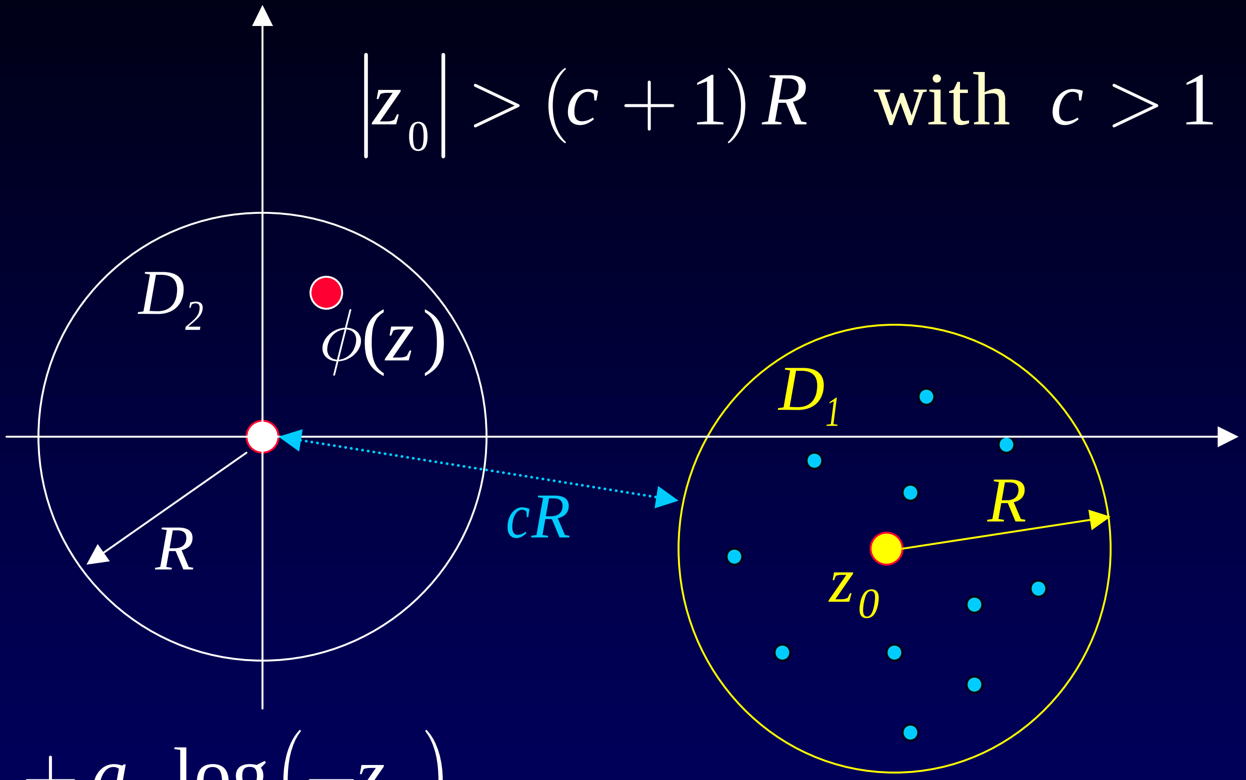
$$\phi(z) \doteq a_0 \log(z) + \sum_{l=1}^{p} \frac{b_l}{z^l}$$ with

$$b_l = \left(\sum_{k=1}^{l} a_k z_0^{l-k} \binom{l-1}{k-1} \right) - \frac{a_0 z_0^l}{l}$$



M2L

$$|z_0| > (c+1)R \quad \text{with} \quad c > 1$$



$$\phi(z) \doteq \sum_{l=0}^{p} b_l \cdot z^l$$

with

$$b_0 \doteq \sum_{k=1}^{p} \frac{a_k}{z_0^k}(-1)^k + a_0 \log(-z_0)$$

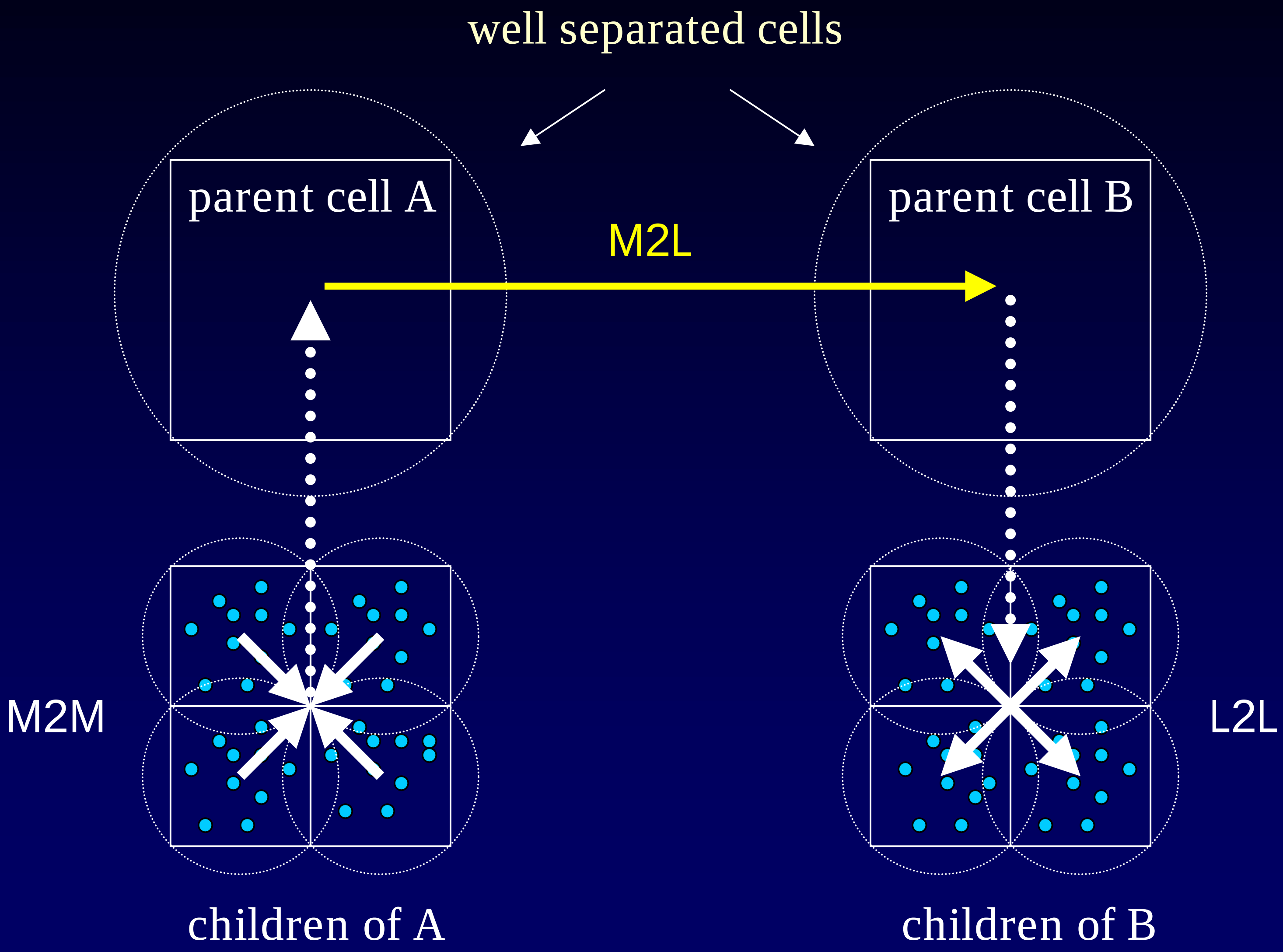
$$b_l \doteq \left(\frac{1}{z_0^l} \sum_{k=1}^{p} \frac{a_k}{z_0^k} \binom{l+k-1}{k-1} (-1)^k \right) - \frac{a_0}{l \cdot z_0^l} \quad \text{for } l \geq 1$$

Shifting a Taylor expansion via an exact translation operation with a finite number of terms:

For any complex $z_0, z,$ and $\{a_k\}, k = 0, \dots, n,$

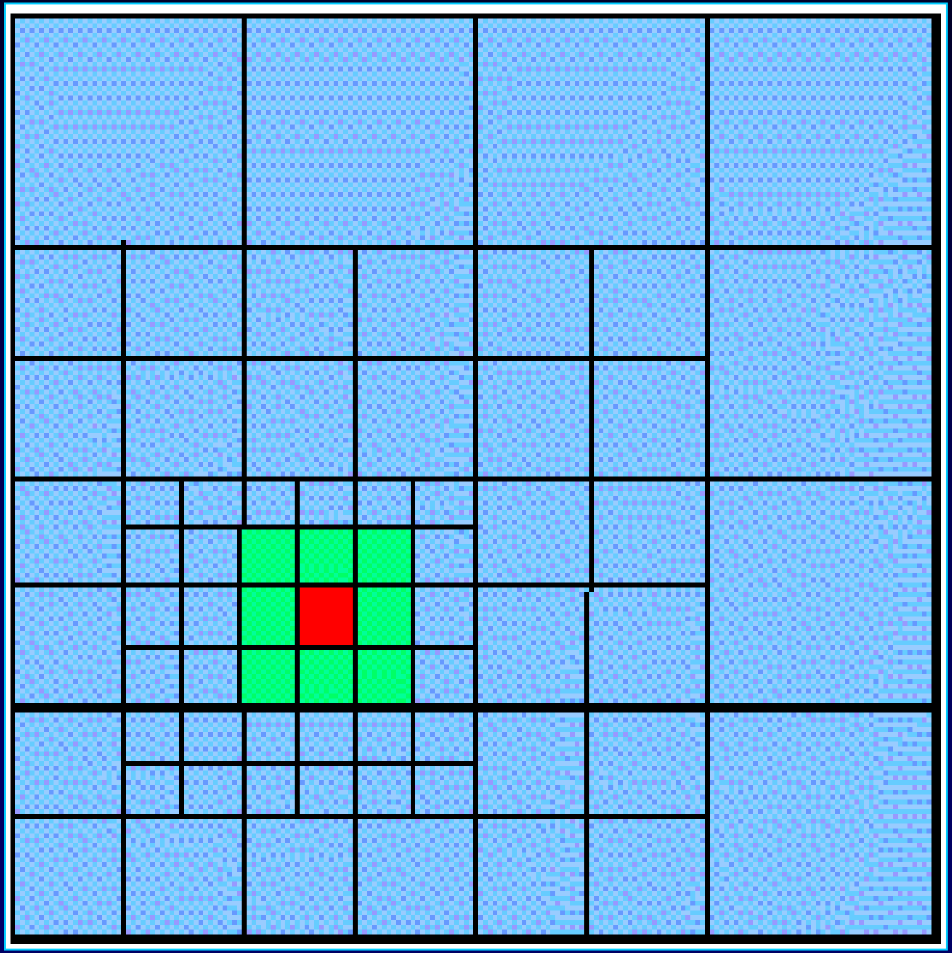
$$\sum_{k=0}^{n} a_k (z - z_0)^k = \sum_{l=0}^{n} \left[\sum_{k=l}^{n} a_k \binom{k}{l} (-z_0)^{k-l} \right] z^l \ .$$

Hierarchy: FMA (1)



Hierarchy: FMA (2)

Levels of refinement



Anderson’s method

- FMM: $\phi(z)$ due to large numbers of particles;
- Not forced to use a multipole expansion as the ‘computational element’.

Instead use Poisson’s formula

Poisson's formula (1)

Solving Laplace's equation for the potential *outside* a disk with radius *a* containing 'sources' :

$$\phi(r,\theta) = \kappa \log(r) +$$

$$\frac{1}{2\pi}\int_{0}^{2\pi}\left(\phi(a,s) - \kappa \log(a)\right)\left[\frac{1-\left(\frac{a}{r}\right)^2}{1-2\left(\frac{a}{r}\right)^2\cos(\theta - s)+\left(\frac{a}{r}\right)^2}\right] ds$$

for $r > a$.

Poisson's formula (2)

... and for the potential *inside* a hole with radius *a* from 'sources' outside:

$$\phi(r,\theta) = \frac{1}{2\pi}\int_0^{2\pi} \phi(a,s)\left[\frac{1-\left(\frac{r}{a}\right)^2}{1-2\left(\frac{r}{a}\right)^2\cos(\theta - s)+\left(\frac{r}{a}\right)^2}\right] ds$$

for $r < a$.

Outer ring approximation (1)

Numerical representation :

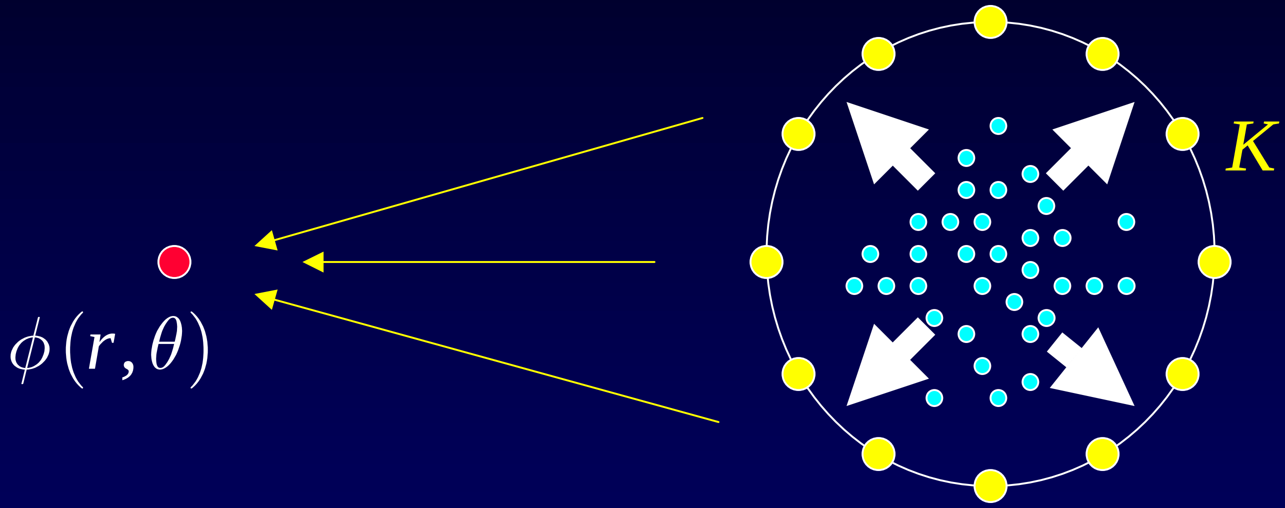
With M an integer and $K = 2M + 1$, we set

$h = 2\pi / K$ and $s_i = \left(a\cos(ih), a\sin(ih)\right),\ i = 1, \ldots, K$:

$$\phi(r,\theta) \doteq \kappa \log(r) +$$

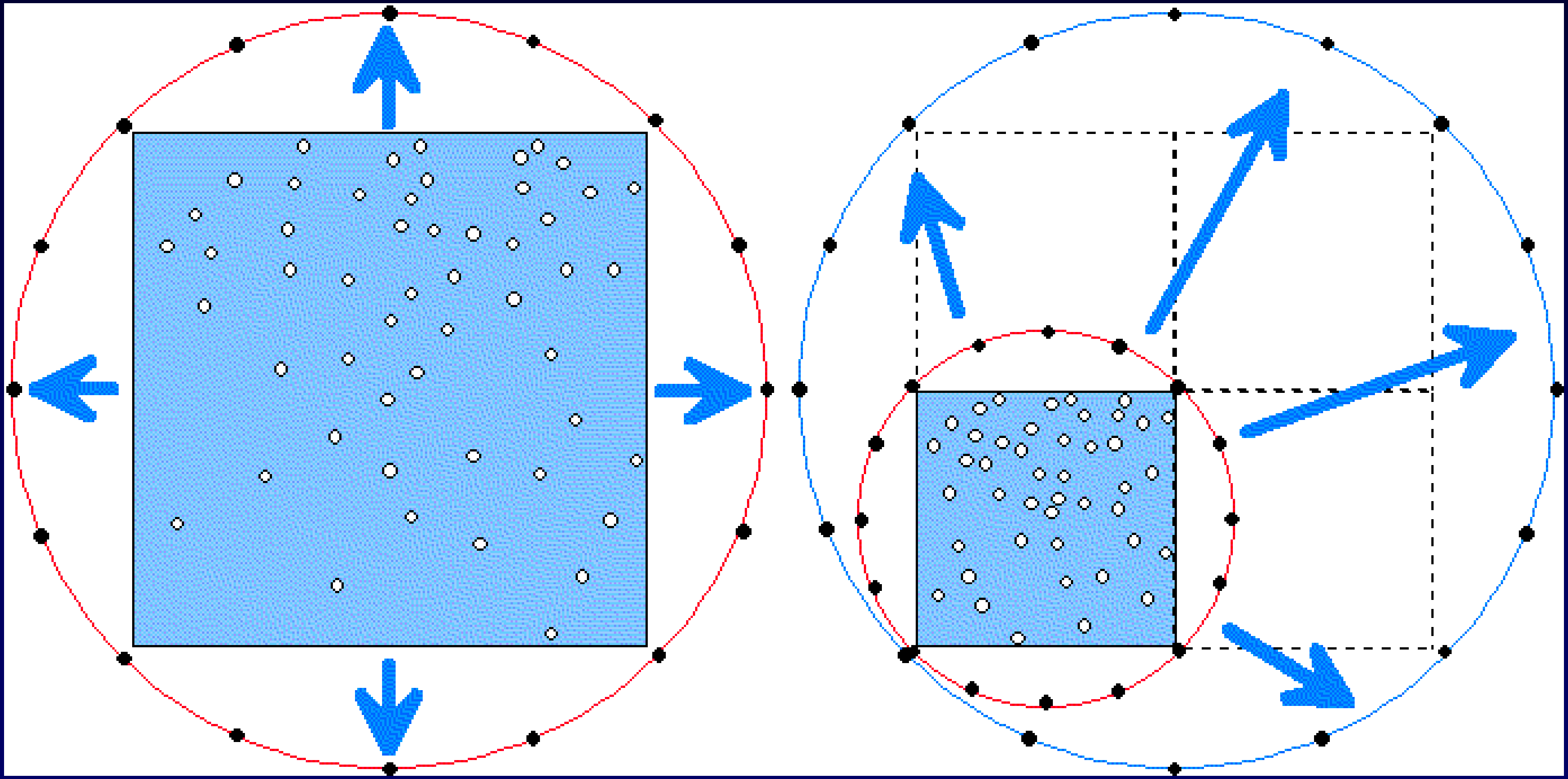
$$\frac{1}{2\pi}\sum_{i=1}^{K}\left(\phi\left(a, s_i\right) - \kappa\log(a)\right)\left[\frac{1-\left(\frac{a}{r}\right)^2}{1-2\left(\frac{a}{r}\right)^2\cos(\theta - s_i) + \left(\frac{a}{r}\right)^2}\right]h$$

Outer ring approximation (2)



Parent outer rings

Construction via Poisson's formula:



Inner ring approximation

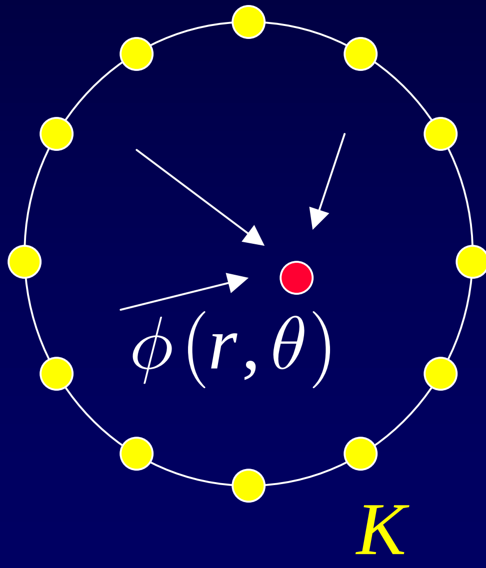
Similar as the outer ring construction:

With M an integer and $K = 2M + 1$, we set

$h = 2\pi / K$ and $s_i = \left(a\cos\left(ih\right), a\sin\left(ih\right)\right),\ i = 1,\ldots,K$:

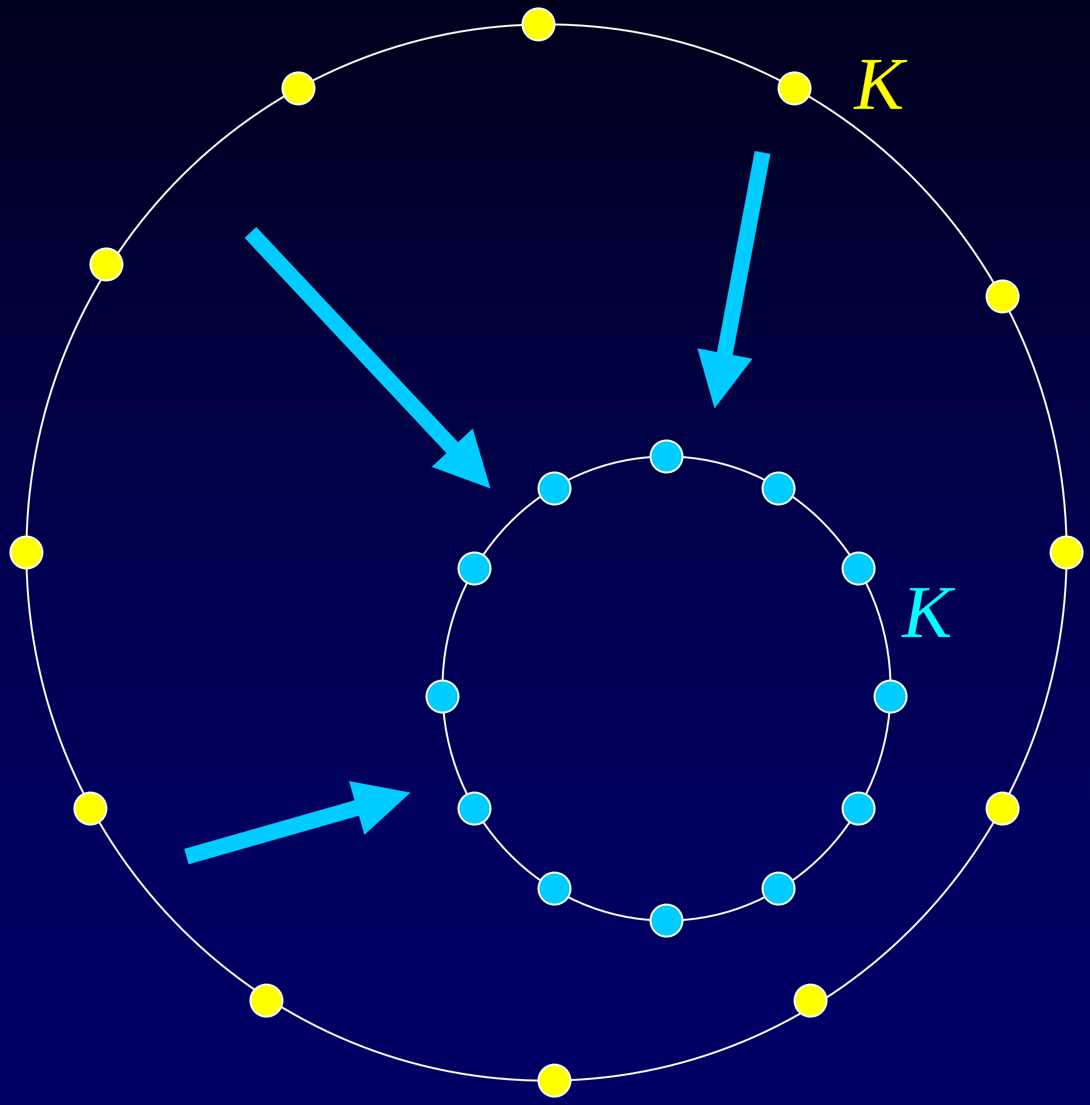
$$\phi\left(r,\theta\right) \doteq$$

$$\frac{1}{2\pi}\sum_{i=1}^{K}\phi\left(a,s_i\right)\left[\frac{1-\left(\frac{a}{r}\right)^2}{1-2\left(\frac{a}{r}\right)^2\cos(\theta - s_i) + \left(\frac{a}{r}\right)^2}\right]h$$



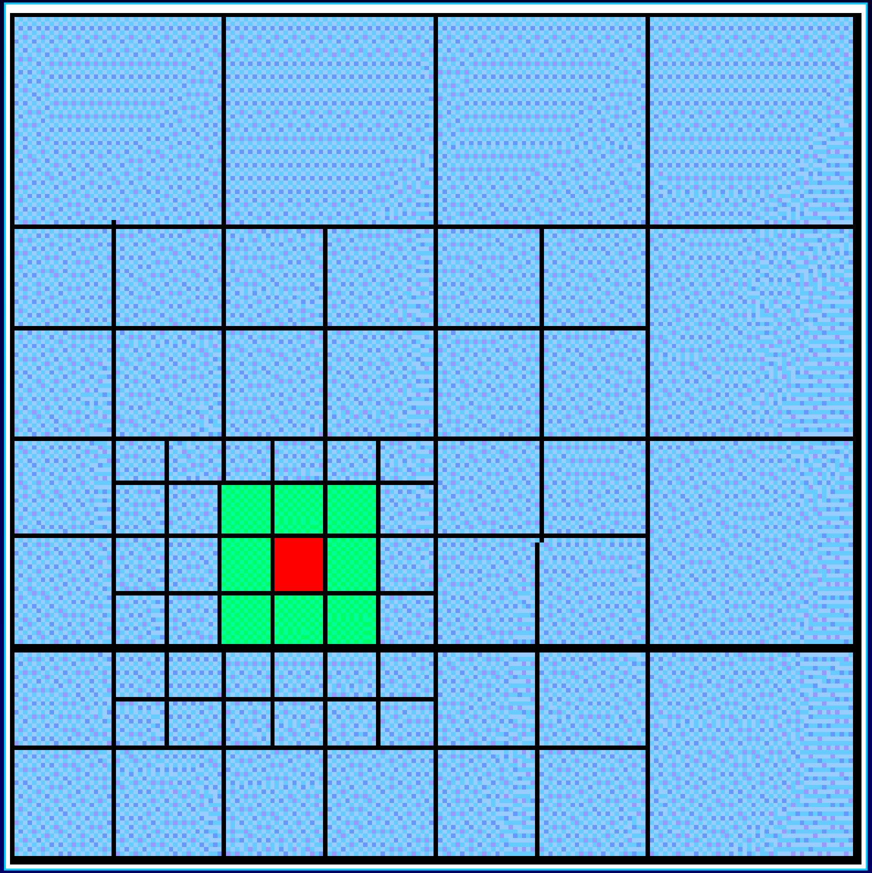
for $r < a$.

Children inner rings

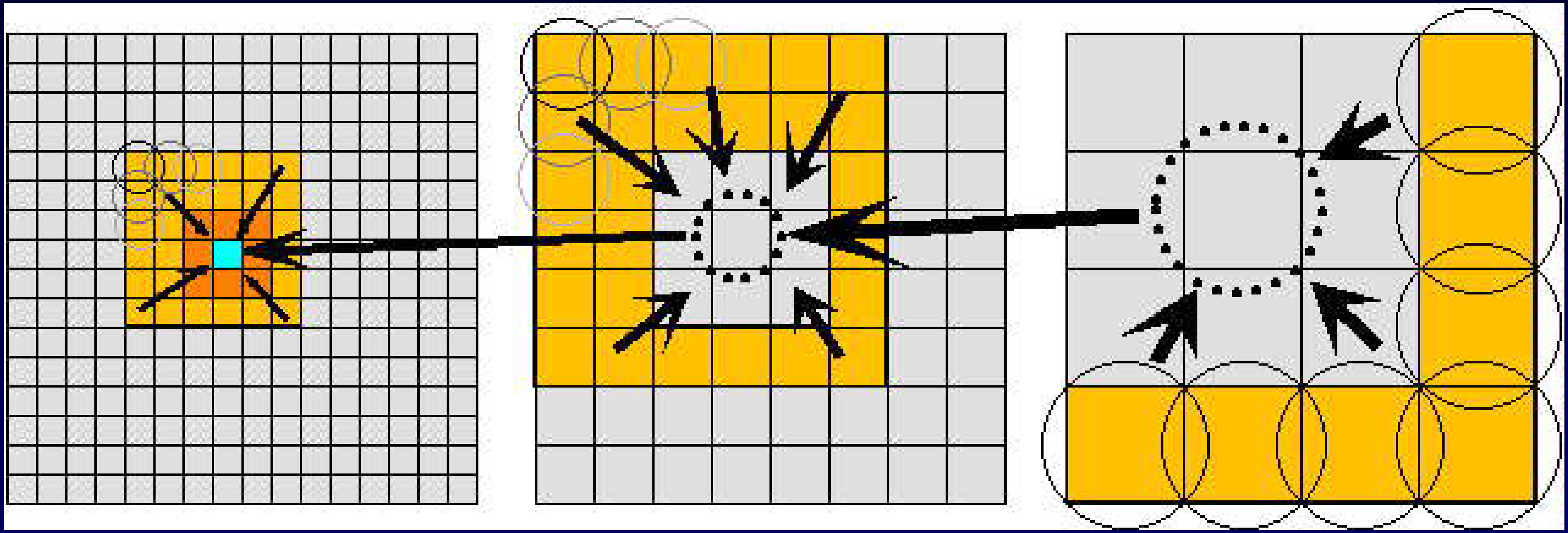


Hierarchical tree

Levels of refinement



Hierarchy in action



Temporal complexity (1)

Seven steps in the hierarchy :

1. Finest level direct interactions $\propto N^2$;
2. Finest level outer ring construction $\propto KN$;
3. Finest level contribution by outer rings in well-separated area $\propto KN$;
4. Outer ring approximations $\propto K^2$;
5. Inner ring approx. by outer rings $\propto K^2$;
6. Inner ring approx. by inner ring parent $\propto K^2$;
7. Finest level contribution by inner ring parent $\propto KN$.

Temporal complexity (2)

- Total operation count depends on l_f, N, and K; with $K << N$ and $l_f = f(N)$;
- For large l_f this leads to :

$$\boxed{\text{Complexity} \sim \alpha 4^{-l_f} N^2 + \beta K N + \gamma 4^{l_f} K^2}$$

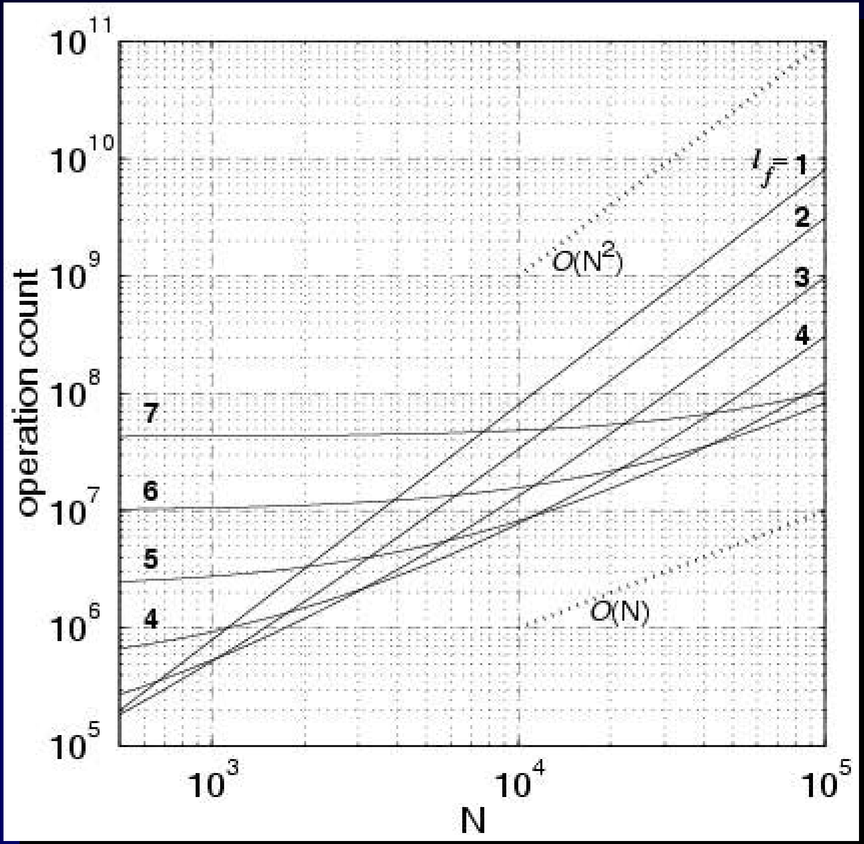
with $\alpha, \beta, \gamma,$ and K of order $O(10)$ for a uniform distribution of particles,

resulting in →

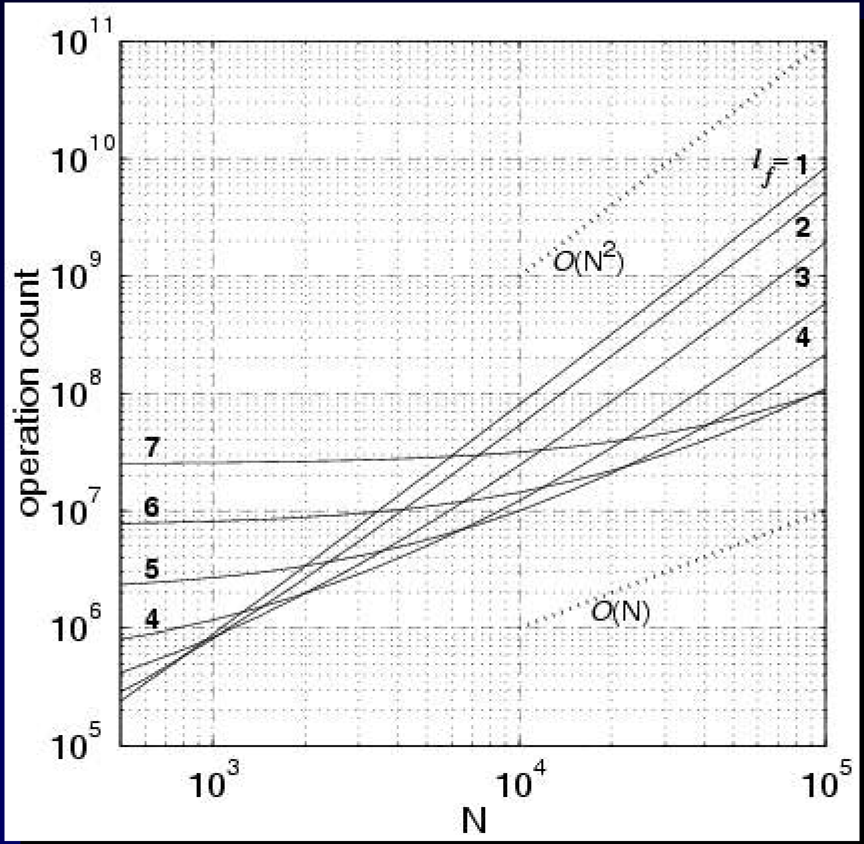
Temporal complexity (3)

an operation count linear in N

Uniform distribution



Non-uniform distribution



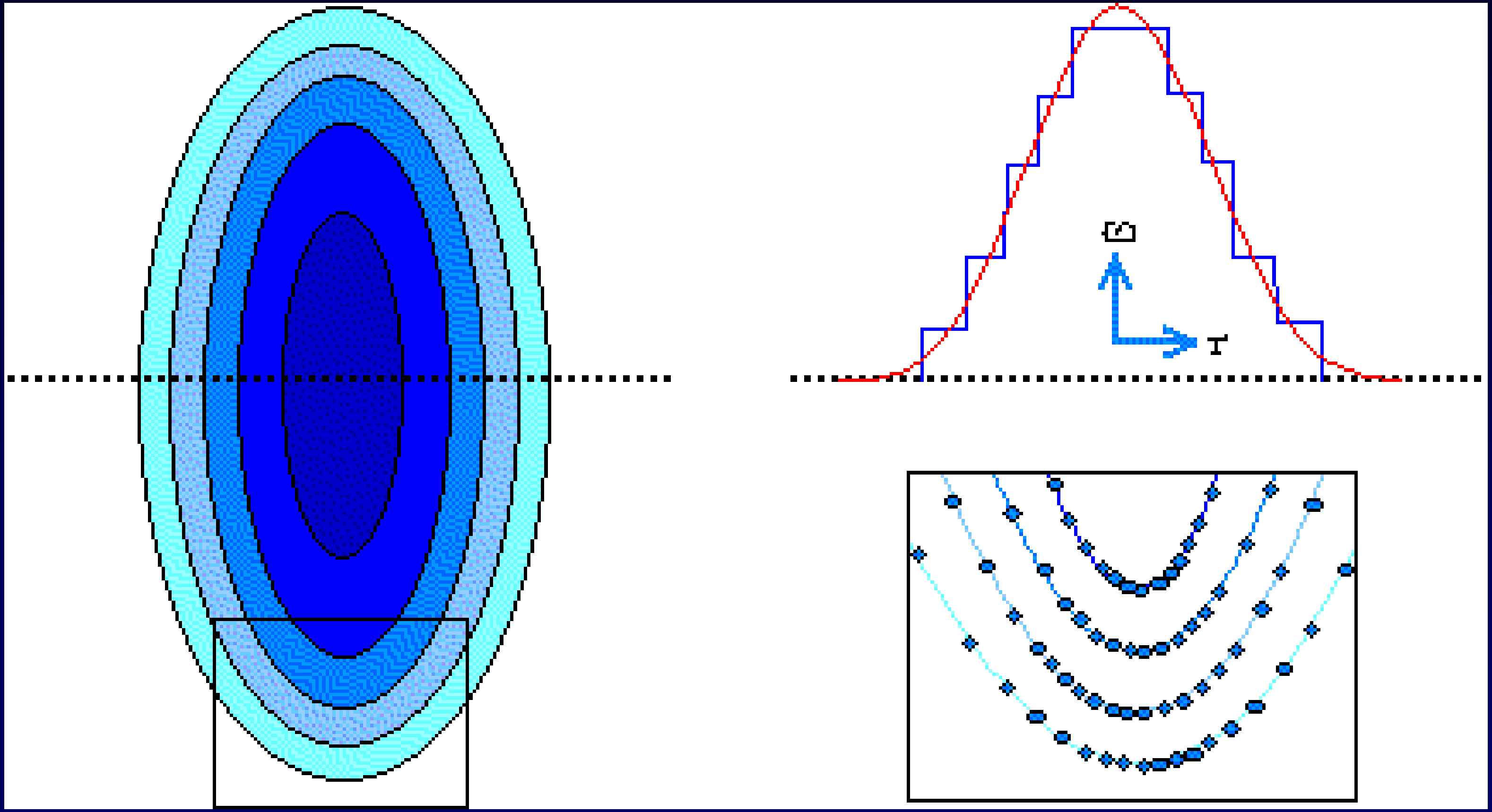
Contour dynamics (1)

Numerical method for simulating :

- 2D, inviscid, incompressible vortex flows;
- Patches of uniform vorticity;
- Velocity field determined by the evolution of the contour bounding the patch:

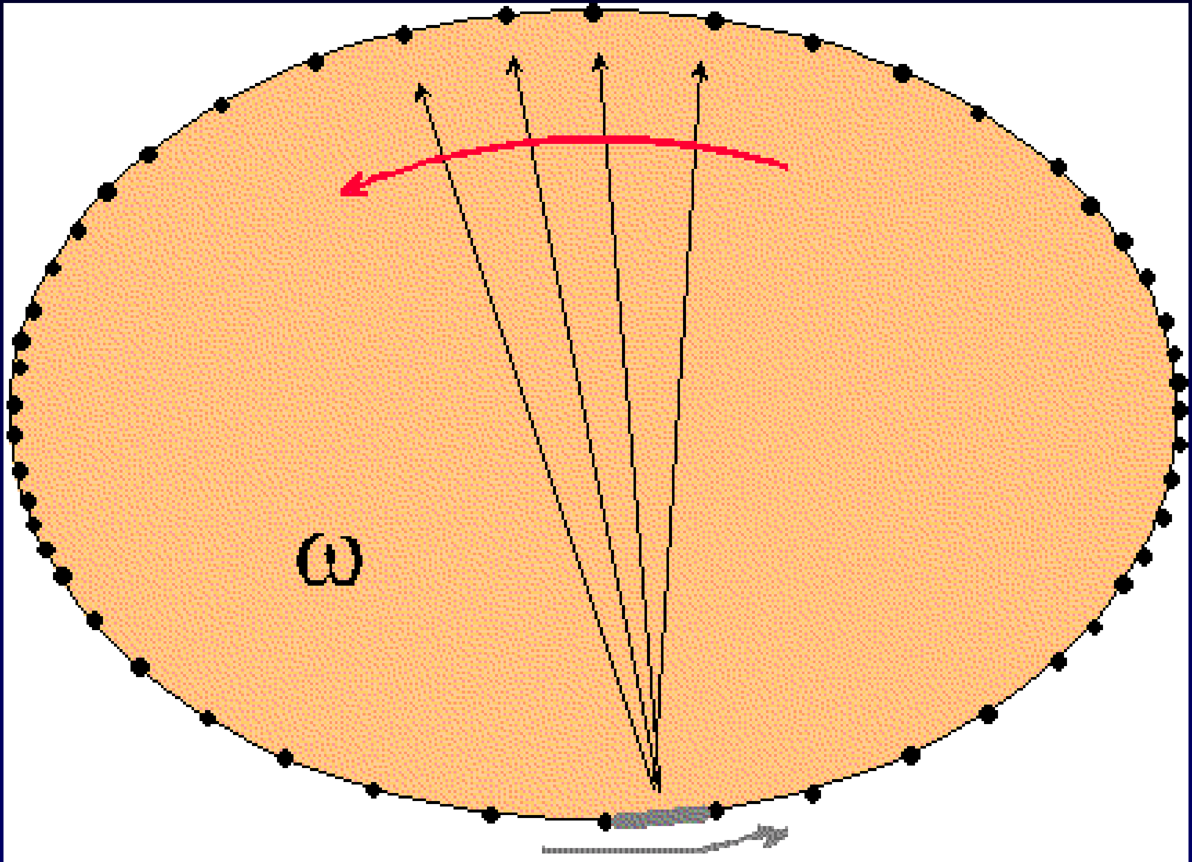
$$\mathbf{u}(\mathbf{r},t) = \oint_{C(t)} \ln|\mathbf{r}-\mathbf{r}'|\,d\mathbf{r}'.$$

Contour dynamics (2)



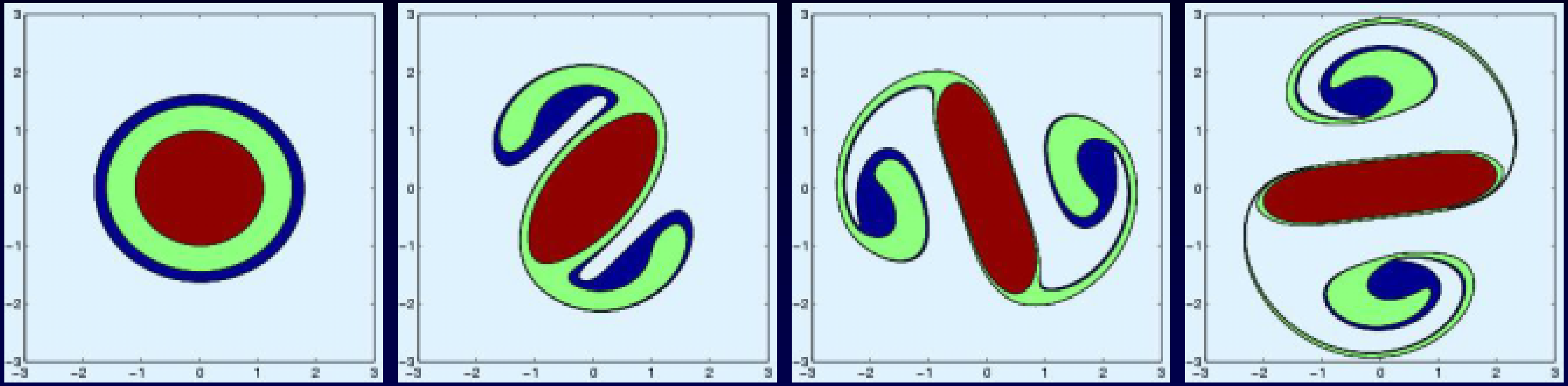
Contour dynamics (3)

An $O(N^2)$ method

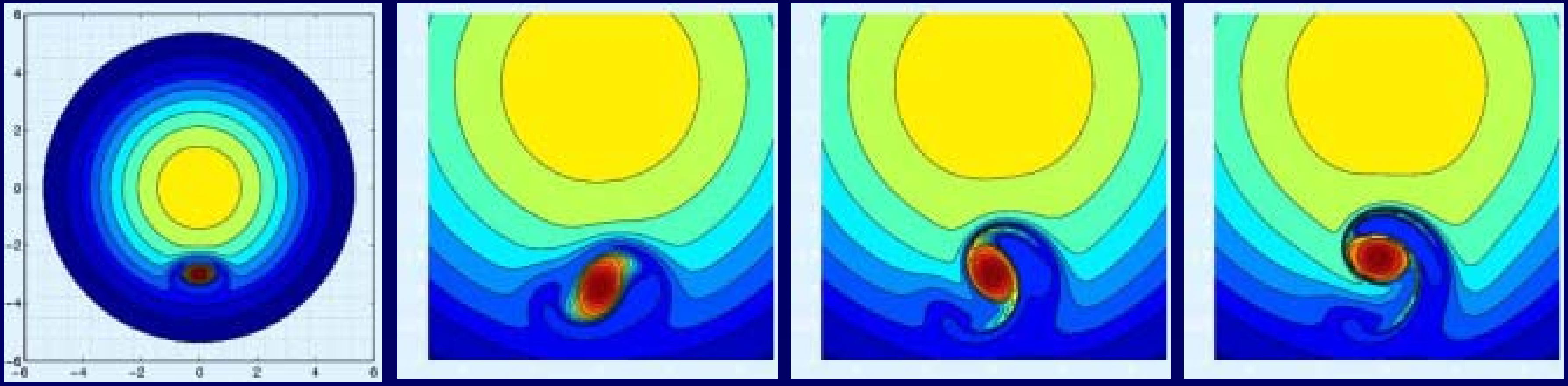


Contour dynamics (4)

- Simple case : $N = O(10^2)$:



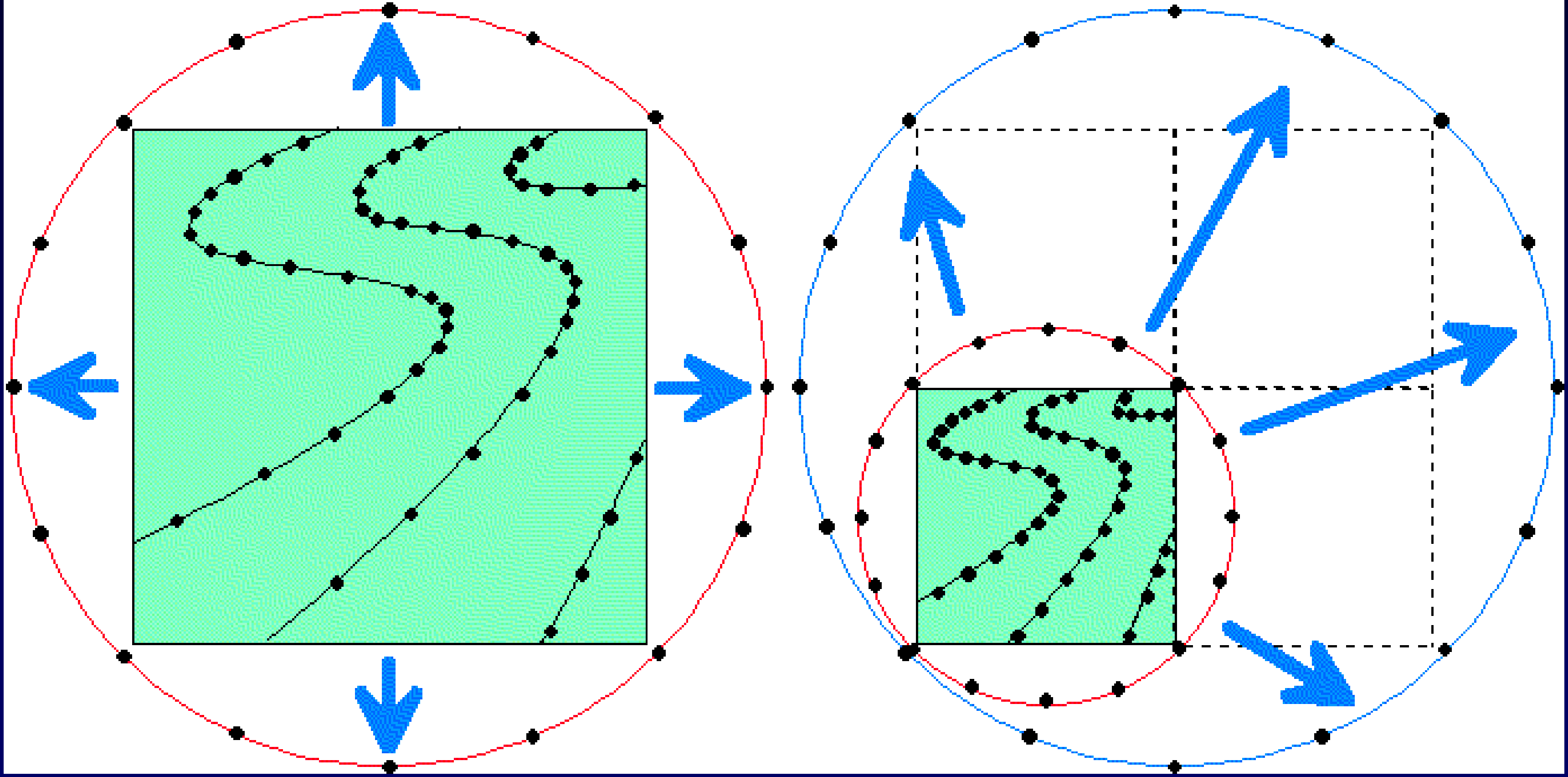
- Hard case : $N = O(10^4)$:



Apply Anderson’s method

Instead of point sources, use

source distributions like vorticity :



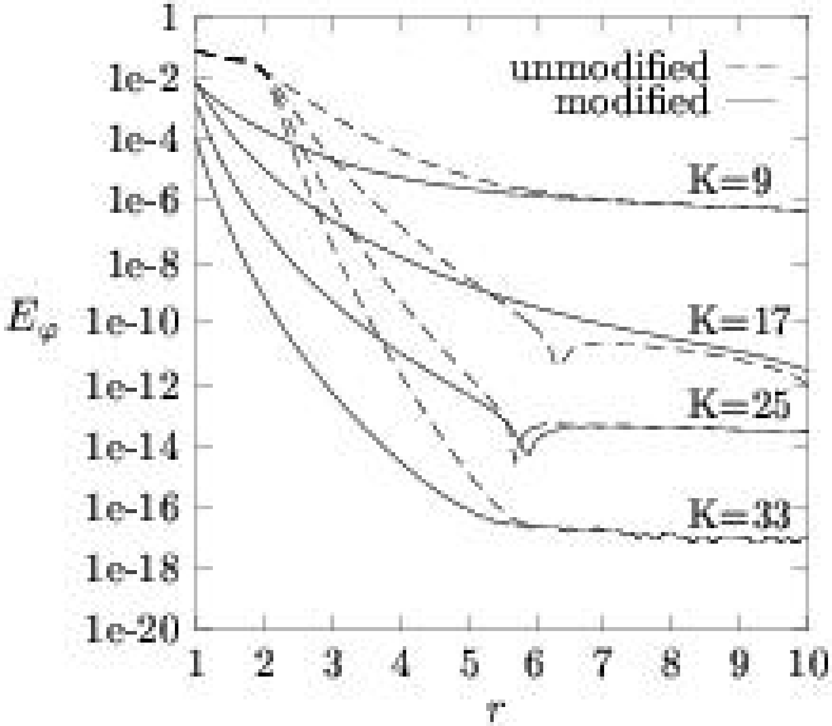
Accuracy of Poisson kernel (1)

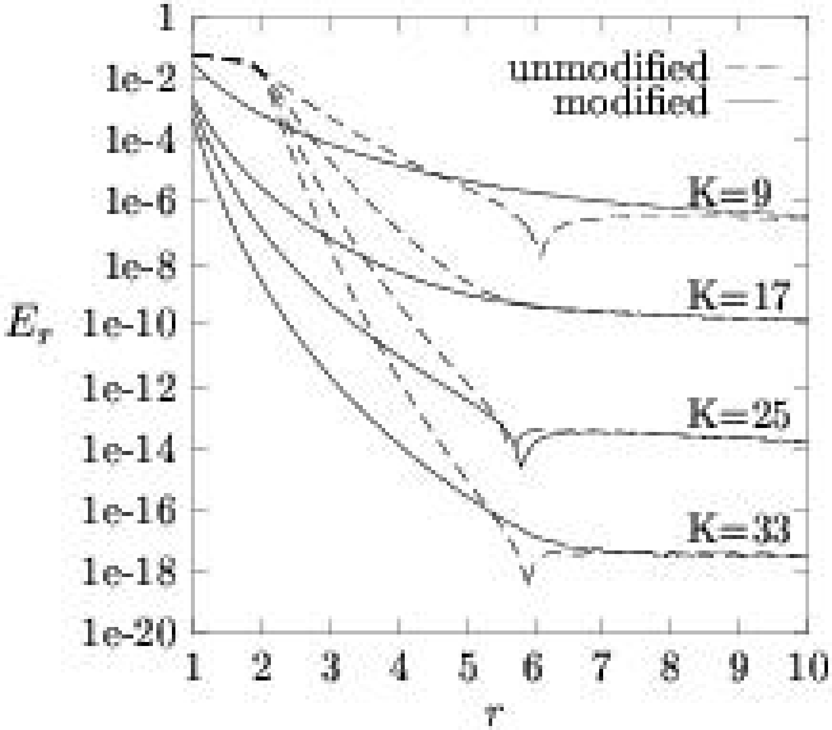
Kernel is very inaccurate for $r \to a$:

$$\phi(r,\theta) \doteq \frac{1}{2\pi} \sum_{i=1}^{K} \phi\left(a, s_i\right) \left[\frac{1 - \left(\frac{a}{r}\right)^2}{1 - 2\left(\frac{a}{r}\right)^2 \cos(\theta - s_i) + \left(\frac{a}{r}\right)^2} \right] h$$

- Anderson solves for this: *C.R. Anderson, SIAM J.Sci.Stat.Comput. Vol 13, No. 4, 1992;*
- Vosbeek solves for this → **HEM** (Hierarchical-Element Method): *P.W.C. Vosbeek et al., J.Comput.Phys., Vol. 161, 2000.*

Accuracy of Poisson kernel (2)





From: *P.W.C. Vosbeek et al., J.Comput.Phys., Vol. 161, 2000.*

Advantages of AM/HEM

- Not only point sources!
- Operations for constructing and combining elements are easy to formulate: only function evaluation;
- These operations are almost identical in 2 and 3 dimensions (not discussed);
- HEM more accurate than AM;
- $O(N)$.