OUTLINE

- DEFINITION ; MOTIVATION
- GRAVITATIONAL n-BODY PROBLEM
- BARNES-HUT TREE ALGORITHM
- PARTICLE MESH TECHNIQUES (PM)
- PARTICLE-PARTICLE, PARTICLE-MESH TECHNIQUES (P^3M)

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DEFINITION: DEFINE BY WHAT PARTICLE HAS, DOESN'T HAVE

HAS: SPACETIME LOCATION, PHYSICAL ATTRIBUTES (MASS, SPIN/ANG. MOM, CHARGE etc)

HASN'T: INTERNAL STRUCTURE - I.E PARTICLES ARE POINT-LIKE ENTITIES

MOTIVATION:

- PARTICLE DESCRIPTIONS / APPROACHES UBIQUITOUS IN PHYSICS / NATURAL SCIENCES
- HUGE FIELD, INCLUDES, e.g., ALL of MOLECULAR DYNAMICS
- FAITHFULNESS of MODELING VIA PARTICLES SPANS WIDE RANGE:
  - SOMETIMES MODELING VERY ACCURATE: e.g. GLOBULAR CLUSTER
  - " " " CONVENIENT: e.g. "MONTE CARLO" INTEGRATION of BOLTZMANN EQUATIONS

* FOR SEVERAL REASONS, INCLUDING TIME CONSTRAINTS WILL FOCUS ON GRAVITATIONAL N-BODY PROBLEM (HW 1, Q2

N PARTICLES: MASSES: $m_i, \; i = 1, \ldots, N$

POSITIONS: $\vec{r}_i(t), \; i = 1 \ldots N$

EQUATIONS of MOTION

$$m_i \ddot{\vec{r}}_i = -G \sum_{\substack{j=1 \\ j \neq i}}^{N} \frac{m_i m_j}{r_{ij}^3} \vec{r}_{ij}$$

$$\dot{q} \equiv \frac{dq}{dt}$$

$$\vec{r}_{ij} \equiv \vec{r}_i - \vec{r}_j$$

$$r_{ij} \equiv \left(\vec{r}_{ij} \cdot \vec{r}_{ij} \right)^{1/2}$$

SOLVE AS INITIAL VALUE PROBLEM, NEED TO SPECIFY 6N INITIAL CONDITIONS

$$\vec{r}_i(0) = \vec{r}_i^{\,0}, \quad i = 1 \ldots N$$

$$\dot{\vec{r}}_i(0) = \vec{v}_i^{\,0}, \quad i = 1 \ldots N$$

OMPUTE SOLUTION ON FINITE TIME INTERVAL $0 \le t \le t_{max}$

INTERESTED IN SCALING of COMPUTATIONAL COST AS FCN of N

- ASSUME LARGE N LIMIT, FIXED INTEGRATION INTERVAL, SPECIFIED LOCAL / GLOBAL ACCURACY
- ISSUE COMPLICATED BY FACT THAT # ~~OF~~ DISCRETE TIME STEPS REQUIRED MAY BE FCN of N

• THIS WILL FOCUS ON PER TIME STEP COMPUTATIONAL COST AND WILL NOT DELVE INTO DETAILS OF TIME INTEGRATION

COST of DIRECT ("BRUTE FORCE") CALCULATION

$$O(N^2)$$

• VERY BAD NEWS FOR LARGE N: MUCH of WHAT FOLLOWS FOCUSES ON ALGORITHMS TO SIGNIFICANTLY IMPROVE ON THIS

PARTICLE-BASED MODELING: PROS / CONS

PROS

1) GRIDLESS, "NATURALLY LAGRANGIAN" - I.E. PARTICLES TEND TO AUTOMATICALLY BE "WHERE THE ACTION IS" (CONTRAST W. DYNAMIC, HIERARCHICAL REGRIDDING IN MESH BASED APPROACHES)
2) TEND TO BE DIMENSIONALLY AGNOSTIC: 3d IMPLEMENTATION NOT SIGNIFICANTLY MORE DIFFICULT THAN 1d
3) INTERACTION OFTEN KNOWN PRECISELY, AND EASY TO COMPUTE FOR ANY GIVEN PAIR of PARTICLES

CONS

1) IN MANY INSTANCES, FOR N > "few", COMP. PROBLEM HAS STOCHASTIC / STATISTICAL ASPECT DUE TO "CHAOTIC" BEHAVIOUR => WILL NEED TO CONSIDER ENSEMBLES of CALCS, CAN EXPECT $N^{-1/2}$ ERROR BEHAVIOUR

- WITH LONG-RANGE INTERACTIONS (GRAVITY, ELECTROSTATICS ...)

FORCE LAWS NON-LOCAL $\Rightarrow$ COMP WORK $\sim N^2$!!

∘ HOWEVER, "NATURE DOESN'T CHOKE AS $N \to \infty$";
SOL^n TO SCALING PROBLEM CAN RATHER GENERALLY
BE VIEWED IN CONTEXT of TAKING "SPACETIME FIELD"
CONCEPT UNDERLYING (MOST) PARTICLE INTERACTIONS
SERIOUSLY $\Rightarrow$ RESTORE FUNDAMENTAL LOCALITY of INTERACTIONS

NOTE: FROM COMP. EFFORT P.O.V. PARTICLE PROBLEMS WITH ONLY SHORT RANGE INTERACTIONS "EASY" - USUALLY STRAIGHTFORWARD TO ACHIEVE $O(N)$ PERFORMANCE, BUT NOTE

- OFTEN STILL HAVE $N^{-1/2}$ ERRORS TO BATTLE, MAY WANT TO CONSIDER "ACC^N STRATEGIES"

- MAY STILL INVOLVE INTERESTING ALGORITHMS (NEIGHBOR LISTS, etc)

NOTE THAT GRAVITATIONAL FORCE IS "WORST CASE" IN SENSE THAT

1) IT IS ∞ RANGE
2) THERE IS NO SCREENING (EXCEPT IN e.g. COSMO. SITUATIONS WHERE FUND QUANTITY IS FLUCTUATION FROM MEAN FIELD $\Rightarrow$ BOTH SIGNS of GRAV MASS)

HEURISTIC ARGUMENT FOR EXISTENCE OF $O(N)$ (!) ALG. FOR GRAV. N-BODY PROBLEM (MWC UNPUBLISHED)

IDEA: WORK TO SOME SPECIFIED PRECISION, ϵ

1) ESCHEW FORCE LAW IN FAVOUR OF COMPUTATION OF $\ddot{\vec{r}}_i$ FROM GRAV. POTENTIAL

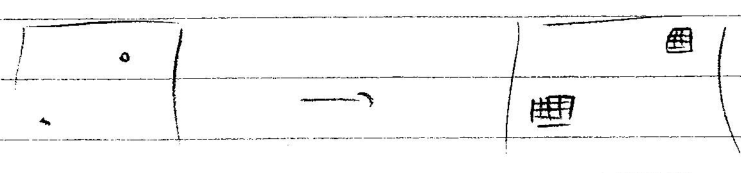
$$\ddot{\vec{r}}_i(t) = \vec{a}(\vec{r}_i, t) = -\vec{\nabla}\phi(\vec{r}_i, t)$$

WHERE GRAV. POTENTIAL SATISFIES

$$\nabla^2 \phi(\vec{r}, t) \propto \rho(\vec{r}, t) \qquad (*)$$

CLEARLY, GIVEN $\phi(\vec{r}, t)$, COMPUTATION OF N INDIVIDUAL ACC^{N}S IS $O(N)$ PROCESS

2) INTRODUCE MESH ON WHICH TO APPROXIMATELY COMPUTE ϕ; MAKE MESH LOCALLY ADAPTIVE SO THAT EACH PARTICLE IS REPRESENTED AS (SMOOTHED) MATTER DISTRIBUTION ON SUFFICIENTLY FINE MESH



FOR GIVEN ϵ, WILL NEED SOME (ROUGHLY) FIXED NUMBER, m, MESH POINTS TO REPRESENT PARTICLE AS SMOOTH CONTRIBUTION TO ρ

3) TOTAL # OF MESH PTS LOCALLY REPRESENTING PARTICLES IS THUS $\sim m N' = O(N)$ (NOTE: m MAY BE [VERY] LARGE !) ; ADDITIONAL GRID PTS REQUIRED TO "FILL IN" BETWEEN PARTICLES WILL ALSO TEND TO BE $O(N)$ — WORST CASE IS UNIFORMLY DISTRIBUTED PARTICLES (MINIMIZES "OVERLAP" OF FINE GRIDS AROUND PARTICLES) — THEN FOR ANY FIXED "COARSE" MESH SPACING, WILL HAVE $O(N)$ PTS

$\Rightarrow$ TOTAL # OF MESH POINTS NEEDED IS $O(N)$

4) MULTI-GRID CAN SOLVE (*) WITH $O(N)$ WORK

5) $\Rightarrow$ TOTAL WORK REQUIRED $O(N)$

AGAIN, m MAY BE SO LARGE THAT N NEEDS TO BE HUGE IN ORDER FOR PROPOSED ALG TO "BEAT" $O(N^2)$ BUT THIS IS IRRELEVANT

WHAT IS RELEVANT IS $N \to \infty$ SCALING, AND THIS ARGUMENT SHOWS THAT IN THAT LIMIT SHOULD GET $O(N)$ SCALING, BASICALLY AS A RESULT of RESTORING FUNDAMENTAL LOCALITY of INTERACTIONS (DESPITE APPEARANCES TO THE CONTRARY)