2010 HIPACC Astro-Computing Summer School

## Galaxy Simulations Using the N-Body/SPH code GADGET

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### Project I.I: Code Optimization

#### PBS batchscript :

#!/bin/sh
#PBS -q batch
#PBS -N Sbc
#PBS -l nodes=2:ppn=2
#PBS -o Sbc.out
#PBS -e Sbc.err
#PBS -V
#PBS -V
#PBS -N tcox@obs.carnegiescience.edu
#PBS -m abe

cd /home/hipacc-5/Sbc/

While you're free to email me, your batch scripts should really contain your email address.

mpirun -v -machinefile \$PBS\_NODEFILE -np 4 ./Gadget2 Sbc.txt > output0.txt

### Outline

- I. Who am I and what am I doing here? My perspective, my science, and where my focus will be this week
- 2. An overview of GADGET projects (+other practical I hope information)
- 3. A brief overview of GADGET
- 4. Adding "Astrophysics" to GADGET
- 5. Loose Ends ... data structures, analysis, and visualization (w/ P. Hopkins)
- 6. What's next? (higher resolution, new models, and Arepo: the next generation of code)

### 3. GADGET: A Brief Intro

- 3.1 The Monte Carlo, N-body approach to solving the CBE
- 3.2 Gravity calculation
- 3.3 Integration and time-steps
- 3.4 Including hydrodynamics with SPH
- 3.5 The steps Gadget takes to accomplish the above
- 3.7 Data Structures within Gadget
- 3.8 Modes of Gadget
- 3.9 The remaining compile-time and run-time parameters
- 3.10 Odd and Ends ... Questions

## Gadget (and other N-body) Resources

- Gadget Manual comes with the public download
- Gadget papers: I (Springel, Yoshida, & White 2000) and 2 (Springel 2005)
- Hernquist & Katz (1989): TreeSPH (basically, Gadget version 0)
- Josh Barnes: (Barnes & Hut 1985, Barnes' website, his 1996 Saas-Fee lectures)
- Volker Spingel's 2009 IAS Summer School lectures (very technical, but a thorough introduction to the nitty-gritty)
- Binney & Tremaine, Galactic Dynamics (1987)
- Hands-on experience digging within the code, modifying it, screwing it up and trying to figure out how to fix it again ....

3.1 Mont Carlo Approach to solving the Collisionless Boltzmann Equation

Galaxies are collisionless systems; t\_relax ~ (N/8LnLambda) t\_cross (see Binney & Tremaine for a nice discussion of this)

**BASIC MONTE-CARLO IDEA** 

Collisionless Boltzmann equation

 $\begin{aligned} \frac{\mathrm{d}f}{\mathrm{d}t} &= \frac{\partial f}{\partial t} + \frac{\partial f}{\partial \mathbf{x}} \cdot \mathbf{v} + \frac{\partial f}{\partial \mathbf{v}} \cdot \left(-\frac{\partial \Phi}{\partial \mathbf{x}}\right) = 0\\ \nabla^2 \Phi(\mathbf{x}, t) &= 4\pi G \int f(\mathbf{x}, \mathbf{v}, t) \,\mathrm{d}\mathbf{v} \end{aligned}$ 

N-body System

$$\begin{split} \ddot{\mathbf{x}}_i &= -\nabla_i \, \Phi(\mathbf{x}_i) \\ \Phi(\mathbf{x}) &= -G \sum_{j=1}^N \frac{m_j}{\left[ (\mathbf{x} - \mathbf{x}_j)^2 + \epsilon^2 \right]^{1/2}} \end{split} \text{ need large}$$

#### 3.1 Mont Carlo Approach to solving the Collisionless Boltzmann Equation



Gravitational softening within some scale accounts for finite N. Gadget uses spline kernel.

ы

0.5

1.0

1.5

-3.0

0.0

What should the gravitational softening be? ..... unfortunately, this isn't an easy question to answer.

\*To zeroth order, collisionless criterion suggest it should depend on N and t\_cross

\* Cosmological simulations often employ simple criterion based upon the mean inter-particle spacing (~1/20th or so)

 $\ast$  Power et al. (2003) present a nice discussion and argue for values based on N and the size of the DM halo

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\* Cosmological simulations often employ simple criterion based upon the mean inter-particle spacing ( $\sim 1/20$ th or so)

\* Power et al. (2003) present a nice discussion and argue for values based on N and the size of the DM halo

While these estimates are useful starting points, there is NO definitive way to know what the softening should be outside of performing detailed numerical experiments. What should the gravitational softening be? ..... unfortunately, this isn't an easy question to answer.

#### Compile-time options from within the Makefile:

0.1 0.2 0.4

OPT += -DUNEQUALSOFTENINGS

#### Parameter file options:

% Softening lengths

MinGasHsmlFractional 0.25

| SofteningGas                 | 0.1 |  |
|------------------------------|-----|--|
| SofteningHalo                | 0.2 |  |
| SofteningDisk                | 0.1 |  |
| SofteningBulge               | 0.1 |  |
| SofteningStars               | 0.1 |  |
| SofteningBndry               | 0.1 |  |
|                              |     |  |
| SofteningGasMaxPhys          |     |  |
| SofteningHaloMaxPhys         |     |  |
| SofteningDiskMaxPhys         |     |  |
| C - Chamin - Duil - Mau Dhua |     |  |

SofteningBulgeMaxPhys 0.1

SofteningStarsMaxPhys 0.1

SofteningBndryMaxPhys 0.1

\*The answer to this question is easy - as large as possible!

\*The answer to this question is easy - as large as possible!

Of course, N\_simulated will always (at least for the near future) be much smaller than N\_actual, so the only way to know what affect the choice of N plays on your results is to perform detailed numerical experiments.

An example:

A current "typical" run (moderately high resolution, but quick enough to run numerous runs) has I million DM particles, 300k gas and collisionless disk particles, and 100k bulge particles. The gravitational softening was 70 pc for all baryonic components and 250 pc for the DM.

-> isolated galaxy evolved for 3 Gyr: 5 days on 8 processors

-> major merger between two of these: 45 days on 32 processors

Highest resolution mergers:

25 million total / I million gas - ~4 months to completion (128 processors)

15 million total / 3 million gas - still running after 6 months (48 processors)

#### 3.3 Gravity calculation



#### **Tree algorithms**

Idea: Use hierarchical multipole expansion to account for distant particle groups

$$\Phi(\mathbf{r}) = -G\sum_{i} \frac{m_i}{|\mathbf{r} - \mathbf{x}_i|}$$

We expand:

$$\frac{1}{|\mathbf{r} - \mathbf{x}_i|} = \frac{1}{|(\mathbf{r} - \mathbf{s}) - (\mathbf{x}_i - \mathbf{s})|}$$

for 
$$|\mathbf{x}_i - \mathbf{s}| \ll |\mathbf{r} - \mathbf{s}|$$
  $\mathbf{y} \equiv \mathbf{r} - \mathbf{s}$ 

and obtain:

$$\frac{1}{|\mathbf{y}+\mathbf{s}-\mathbf{x}_i|} = \frac{1}{|\mathbf{y}|} - \frac{\mathbf{y} \cdot (\mathbf{s}-\mathbf{x}_i)}{|\mathbf{y}|^3} + \frac{1}{2} \frac{\mathbf{y}^T \left[3(\mathbf{s}-\mathbf{x}_i)(\mathbf{s}-\mathbf{x}_i)^T - \mathbf{I}(\mathbf{s}-\mathbf{x}_i)^2\right] \mathbf{y}}{|\mathbf{y}|^5} + \dots$$

the dipole term vanishes when summed over all particles in the group



### The multipole moments are computed for each node of the tree

Monpole moment:

$$M = \sum_{i} m_{i}$$

Quadrupole tensor:

$$Q_{ij} = \sum_{k} m_k \left[ 3(\mathbf{x}_k - \mathbf{s})_i (\mathbf{x}_k - \mathbf{s})_j - \delta_{ij} (\mathbf{x}_k - \mathbf{s})^2 \right]$$

Resulting potential/force approximation:

$$\Phi(\mathbf{r}) = -G\left[\frac{M}{|\mathbf{y}|} + \frac{1}{2}\frac{\mathbf{y}^{T}\mathbf{Q}\,\mathbf{y}}{|\mathbf{y}|^{5}}\right]$$

For a single force evaluation, not *N* single-particle forces need to be computed, but **only of order** *log(N)* **multipoles**, depending on the opening angle.

- The tree algorithm has no intrinsic restrictions for its dynamic range
- · force accuracy can be conveniently adjusted to desired level
- the speed does depend only very weakly on clustering state
- geometrically flexible, allowing arbitrary geometries

#### 3.3 Gravity calculation

Gadget2 can also calculate gravitational forces via the TreePM method.



#### 3.3 Gravity calculation

#### Compile-time options from within the Makefile:

#----- TreePM Options
#OPT += -DPMGRID=128
#OPT += -DPLACEHIGHRESREGION=3
#OPT += -DENLARGEREGION=1.2
#OPT += -DASMTH=1.25
#OPT += -DRCUT=4.5

#### Parameter file options:

% Tree algorithm, force accuracy, domain update frequency

ErrTolTheta0.5TypeOfOpeningCriterion1ErrTolForceAcc0.005

TreeDomainUpdateFrequency 0.1

Leapfrog integrator (requires a single force computation, conserves phase space/symplectic, and is time reversible)

$$\begin{array}{ll} \mathbf{r}_{n+1/2} &= \mathbf{r}_n + \frac{1}{2} \tau \mathbf{v}_n, & \text{drift} \\ \mathbf{v}_{n+1} &= \mathbf{v}_n + \tau \mathbf{a}(\mathbf{r}_{n+1/2}), & \text{kick} \\ \mathbf{r}_{n+1} &= \mathbf{r}_{n+1/2} + \frac{1}{2} \tau \mathbf{v}_{n+1}, & \text{drift} \end{array}$$

see Quinn et al. (1997) for much more detail and a much better description









the situation can improved with timesteps chosen in a factor of 2 hierarchy, see, e.g., Quinn et al. (1997)

#### Compile-time options from within the Makefile:

#----- Time integration options
OPT += -DSYNCHRONIZATION
#OPT += -DFLEXSTEPS
#OPT += -DPSEUDOSYMMETRIC
#OPT += -DNOSTOP\_WHEN\_BELOW\_MINTIMESTEP
#OPT += -DNOPMSTEPADJUSTMENT

#### Parameter file options:

% Accuracy of time integration

| ErrTolIntAccuracy                  | 0.0025      | $\Delta t_{\rm grav} = \min\left[\Delta t_{\rm max}, \left(\frac{2\eta\epsilon}{ \boldsymbol{a} }\right)^{1/2}\right]$ |
|------------------------------------|-------------|--|
| CourantFac                         | 0.15        |  |
| MaxSizeTimestep<br>MinSizeTimestep | 0.01<br>0.0 | $\Delta t_i^{(\text{hyd})} = \frac{C_{\text{courant}} h_i}{\max_j (c_i + c_j - 3w_{ij})}$                              |

#### Compile-time options from within the Makefile:

#----- Time integration options
OPT += -DSYNCHRONIZATION
#OPT += -DFLEXSTEPS
#OPT += -DPSEUDOSYMMETRIC
#OPT += -DNOSTOP\_WHEN\_BELOW\_MINTIMESTEP
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#----- Time integration options
OPT += -DSYNCHRONIZATION
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#OPT += -DNOSTOP\_WHEN\_BELOW\_MINTIMESTEP
#OPT += -DNOPMSTEPADJUSTMENT

#### Parameter file options:

# Be Careful with this default value!

$$\Delta t_{\text{grav}} = \min\left[\Delta t_{\text{max}}, \left(\frac{2\eta\,\epsilon}{|\boldsymbol{a}|}\right)^{1/2}\right]$$

$$\Delta t_i^{(\text{hyd})} = \frac{C_{\text{courant}} h_i}{\max_j (c_i + c_j - 3w_{ij})}$$

% Accuracy of time integration

| < | ErrTolIntAccuracy                  | 0.0025      | > |
|---|------------------------------------|-------------|---|
|   | CourantFac                         | 0.15        |   |
|   | MaxSizeTimestep<br>MinSizeTimestep | 0.01<br>0.0 |   |



#### cautionary tale:



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# When looking at structure at/near your resolution limit, you need high integration accuracy!

\* Nice discussion from Tom Abel yesterday about various perils of SPH and the new formulation rpSPH

\* And from Tom Quinn this morning ..... so this will be brief. Kernel interpolant of an arbitrary function:

$$\langle A(\mathbf{r}) \rangle = \int W(\mathbf{r} - \mathbf{r}', h) A(\mathbf{r}') \,\mathrm{d}^3 r'$$



This leads to the SPH density estimate, for 
$$A_i = 
ho_i$$
  $ho_i = \sum_{j=1}^N m_j W(|\mathbf{r}_{ij}|,h_i)$ 



#### Smoothed estimate for the velocity field:

$$\langle \mathbf{v}_i \rangle = \sum_j \frac{m_j}{\rho_j} \mathbf{v}_j W(\mathbf{r}_i - \mathbf{r}_j)$$

Velocity divergence can now be readily estimated:

$$abla \cdot \mathbf{v} = 
abla \cdot \langle \mathbf{v}_i 
angle = \sum_j rac{m_j}{
ho_j} \, \mathbf{v}_j \, 
abla_i W(\mathbf{r}_i - \mathbf{r}_j)$$

#### But alternative (and better) estimates are possible also:

Invoking the identity

$$\rho \nabla \cdot \mathbf{v} = \nabla \cdot (\rho \mathbf{v}) - \mathbf{v} \cdot \nabla \rho$$

one gets a "pair-wise" formula:

$$\rho_i (\nabla \cdot \mathbf{v})_i = \sum_j m_j (\mathbf{v}_j - \mathbf{v}_i) \, \nabla_i W(\mathbf{r}_i - \mathbf{r}_j)$$

#### 3.4 Including hydrodynamics via SPH



As both Tom Abel and Tom Quinn have mentioned, there are many formulations of SPH, specifically how you symmetrize the Kernel or the pressure terms.

Gadget uses an entropy formulation derived with a variational approach that alleviates some of the problems associated with varying smoothing lengths (see Springel & Hernquist 2002).

Parameter file options:

% Further parameters of SPH

| DesNumNgb            | 50   |
|----------------------|------|
| MaxNumNgbDeviation   | 2    |
| ArtBulkViscConst     | 0.8  |
| InitGasTemp          | 0    |
| MinGasTemp           | 0    |
| MinGasHsmlFractional | 0.25 |

A brief outline of the modules that Gadget uses to perform the aforementioned processes:



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#### computes accelerations

(accel.c)

- compute gravitational acceleration in gravtree.c
- determine SPH density in density.c
- compute hydrodynamic forces in hydra.c



It is fairly straightforward to add a fixed potential to a Gadget simulation:

\* gravtree.c/gravity\_tree walks tree to compute the gravitational acceleration for each particle and stores this in P[i].GravAccel[j]

\* Loop through the particle a second time and add any additional acceleration you desire.

#### computes accelerations

(accel.c)

- compute gravitational acceleration in gravtree.c
- determine SPH density in density.c
- compute hydrodynamic forces in hydra.c
  - other forces or energies can be included (cooling, star formation feedback, etc.)

There are three primary data structures within Gadget

\*All.(xx) = global variables stored on ALL processors

\* P[i].Pos[j],Vel[j], ..... = particle information, unique to each processor

\* SphP[i].Entropy,Pressure, ...= SPH particle information, unique to each processor

=> see allvars.h for a complete listing of all structure variables
Makefile and parameter settings that need to be changed:

# Compile-time options from within the Makefile:

#OPT += -DPERIODIC

#### Parameter file options:

| ComovingIntegrationOn | 0   |
|-----------------------|-----|
| PeriodicBoundariesOn  | 0   |
| Omega0                | 0   |
| OmegaLambda           | 0   |
| OmegaBaryon           | 0   |
| HubbleParam           | 1.0 |
| BoxSize               | 0   |

|    | Type of Simulation  | I          | Computational methods   | Remarks  |
|----|---|------------|---|--|
| 1  | Newtonian space   |            | Gravity: Tree, SPH<br>(optional), vacuum<br>boundary conditions                               | OmegaLambda<br>should be set to zero   |
| 2  | Periodic long box   |            | No gravity, only SPH,<br>periodic boundary<br>conditions                                      | NOGRAVITY needs to<br>be set, LONG_X/Y/Z<br>may be set to scale the<br>dimensions of the box |
| 3  | Cosmological, physi-<br>cal coordinates                   | Q.         | Gravity: Tree, SPH, vacuum boundaries   | ComovingIntegrationOn<br>set to zero   |
| 4  | Cosmological, co-<br>moving coordinates                   | $\bigcirc$ | Gravity: Tree, SPH, vacuum boundaries   | ComovingIntegrationOn<br>set to one  |
| 5  | Cosmological, co-<br>moving periodic<br>box               |            | Gravity: Tree with<br>Ewald-correction,<br>SPH, periodic bound-<br>aries                      | PERIODIC needs to be set   |
| 6  | Cosmological, co-<br>moving coordinates,<br>TreePM        | $\bigcirc$ | Gravity: Tree with<br>long range PM, SPH,<br>vacuum boundaries                                | PMGRID needs to be<br>set  |
| 7  | Cosmological, co-<br>moving periodic box,<br>TreePM       |            | Gravity: Tree with<br>long range PM, SPH,<br>periodic boundaries                              | PERIODIC and PM-<br>GRID need to be set  |
| 8  | Cosmological, co-<br>moving coordinates,<br>TreePM, Zoom  |            | Gravity: Tree with<br>long-range and<br>intermediate-range<br>PM, SPH, vacuum<br>boundaries   | PMGRID and PLACE-<br>HIGHRESREGION<br>need to be set   |
| 9  | Cosmological, peri-<br>odic comoving box,<br>TreePM, Zoom |            | Gravity: Tree with<br>long-range and<br>intermediate-range<br>PM, SPH, periodic<br>boundaries | PERIODIC, PMGRID<br>and PLACEHIGHRES-<br>REGION need to be set                               |
| 10 | Newtonian space,<br>TreePM                                |            | Gravity: Tree with<br>long-range PM, SPH,<br>vacuum boundaries                                | PMGRID needs to be<br>set  |

Compile-time options from within the Makefile:

- OPT += -DPEANOHILBERT
- OPT += -DWALLCLOCK
- OPT += -DDOUBLEPRECISION
- #OPT += -DDOUBLEPRECISION\_FFTW
- #OPT += -DHAVE\_HDF5
- OPT += -DOUTPUTPOTENTIAL
- #OPT += -DOUTPUTACCELERATION
- #OPT += -DOUTPUTCHANGEOFENTROPY
- #OPT += -DOUTPUTTIMESTEP



Compile-time options from within the Makefile:

OPT += -DPEANOHILBERT

The space-filling Hilbert curve can be readily generalized to 3D THE PEANO-HILBERT CURVE



#### 3.9 The remaining parameters

The remainder of Gadget compile-time and parameter file options .....

Compile-time options from within the Makefile:

OPT += -DPEANOHILBERT





GADGET-3 uses a spacefilling Peano-Hilbert curve which is more flexible EXAMPLE OF DOMAIN DECOMPOSITION IN GADGET-3





# 3.9 The remaining parameters

#### The remainder of Gadget compile-time and parameter file options .....

# Parameter file options:

#### % Relevant files

| InitCondFile<br>OutputDir                         | /home/hipacc-5/MakeDiskGalaxy/Sa.dat<br>/home/hipacc-5/Sa/ |                |        |            |  |
|---|--|----------------|--------|------------|--|
| EnergyFile<br>InfoFile<br>TimingsFile<br>CpuFile  | energy.txt<br>info.txt<br>timings.txt<br>cpu.txt           |                |        |            |  |
| RestartFile restart<br>SnapshotFileBase snapshot  |  |                |        |            |  |
| OutputListFilename parameterfiles/output_list.txt |  |                |        |            |  |
| % Output frequency                                |  |                |        |            |  |
| TimeBetSnapshot 0.05<br>TimeOfFirstSnapshot 0     |  |                |        |            |  |
| CpuTimeBetResta<br>TimeBetStatisti                |  | 1800.0<br>0.05 | ; here | in seconds |  |
| NumFilesPerSnap<br>NumFilesWritten                |  | 1<br>1         |        |            |  |

# 3.9 The remaining parameters

The remainder of Gadget compile-time and parameter file options .....

# Parameter file options:

| % Relevant files  |   |                |               |         |   |            |
|---|---|----------------|---------------|---------|---|------------|
| InitCondFile<br>OutputDir   | /home/hipad<br>/home/hipad  |                | kGalaxy/Sa.da | at      |   |            |
| EnergyFile<br>InfoFile<br>TimingsFile<br>CpuFile<br>RestartFile<br>SnapshotFileBase | energy.txt<br>info.txt<br>timings.txt<br>cpu.txt<br>restart<br>snapshot |                |               |         | → |            |
| OutputListFilename  | -   |                | list tut      |         |   |            |
| % Output frequer  |   |                |               |         | → | checkpoint |
| TimeBetSnapshot   | 0.  | 05             |               |         |   |            |
| TimeOfFirstSnaps  | shot 0  |                |               |         |   |            |
| CpuTimeBetRestar<br>TimeBetStatistic  |   | 1800.0<br>0.05 | ; here in     | seconds |   |            |
| NumFilesPerSnaps<br>NumFilesWrittenI  |   | 1<br>1         |               |         |   |            |

# Restarting from a Checkpoint

#### PBS batchscript :

```
#!/bin/sh
#PBS -q batch
#PBS -N Sbc
#PBS -l nodes=2:ppn=2
#PBS -o Sbc.out
#PBS -o Sbc.out
#PBS -e Sbc.err
#PBS -V
#PBS -M tcox@obs.carnegiescience.edu
#PBS -m abe
cd /home/hipacc-5/Sbc/
mpirun -v -machinefile $PBS_NODEFILE -np 4 ./Gadget2 Sbc.txt > output0.txt
add a "1" to restart from the last
checkpoint - or you can add "2" to start
from the last snapshot, but changes are
also needed in the parameter file too
```

#### Parameter file options:

% CPU time -limit

TimeLimitCPU 36000 % = 10 hours ResubmitOn 0 ResubmitCommand my-scriptfile

#### Parameter file options:

ICFormat11With#OPT+=-DHAVE\_HDF5SnapFormat111111

#### % Caracteristics of run

| TimeBegin | 0.0 | % Begin of the simulation |
|-----------|-----|---------------------------|
| TimeMax   | 1.0 | % End of the simulation   |

#### Parameter file options:

% Memory allocation

PartAllocFactor3.5TreeAllocFactor1.5BufferSize50% in MByte

% System of units

| UnitLength_in_cm         | 3.085678e21 | ; | 1.0 kpc             |
|--------------------------|-------------|---|---------------------|
| UnitMass_in_g            | 1.989e43    | ; | 1.0e10 solar masses |
| UnitVelocity_in_cm_per_s | 1e5         | ; | 1 km/sec            |
| GravityConstantInternal  | 0           |   |                     |

Questions?

How are any tests going?