http://wwwmpa.mpa-garching.mpg.de/galform/data_vis/index.shtml#movie8



HPC challenges in simulation Cosmological Struture Formation

Klaus Dolag, Universitäts Sternwarte München



What do we aim for ?

My God...



...it's full of stars Dave (2001: Space Odyssee): "My God, it's full of stars !"

Bild: APOD 23. Aug 2010, Alex Cherney, Terrastro

What do we aim for ?

Not only, but it is even full of galaxies !

Galaxies show us even the dynamic of the universe !



Bild: NASA, ESA, M.J. Jee and H. Ford

Bild: APOD 21. Juli 2008, Gemini Observatory

How many stars / galaxies ?

~10²², so ca. the numbers of atoms in a dice. Impossible to dircetly simulate !

Photo: Robert Gendler

Stars (200.000.000.000) Galaxies (100.000.000.000)

Bild: APOD 23. Aug 2010, Alex Cherney, Terrastro

Importance of Galaxy Clusters

Ein merkwürdiger Haufen von Nebelflecken.

Auf zwei mit dem Bruce-Teleskop genommenen Aufnahmen vom 24. März dieses Jahres, welche die Umgebung von 31 Comae Berenices darstellen, findet sich eine sehr interessante Gegend des Himmels. Um die Stelle

 $\alpha = 12^{h} 52^{m} 6$ $\delta = +28^{\circ} 42' (1855.0)$

stehen nämlich zahlreiche kleine Nebelflecken so dicht beisammen, dass man beim Anblick der Gegend förmlich über das merkwürdige Aussehen dieses »Nebelhaufens« erschrickt.

Heidelberg, 1901 März 27.

Ich habe die Anzahl der Nebel in einem Kreis von 30' Durchmesser um die angegebene Stelle bestimmt und finde, dass mindestens 108 Nebelflecken auf dieser Fläche beisammen stehen, also auf einer Fläche etwa von der Grösse des Vollmondes. Darunter sind vier oder fünf grössere ausgedehnte und centralverdichtete Nebel, sowie mehrere langgestreckte. Die weitaus meisten haben aber rundliche Form und sind kleiner. *)

Max Wolf.

		o ^m 5	9 ^m 5	8 ¹¹¹ 57	^w 56 ^w	55 ^m	54 ^m 5	53 ^m 5	52 ^m 5	1 ⁿⁱ 50	o ^m 49	9 ¹¹¹ 48	3 ¹¹¹ 47	^{.10} 46	^m 45	^m 44	^m 43	¹⁰ 42	^m 41	¹⁰ 40	o ⁿⁱ 39	9 ^m 3	3 ⁷¹¹ 37	7 ^m 3'	6 ^m 3	.m.	
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64° 0	/-	-	-	0	2	0	1 4	I	I	I	6	4	2	0	0	5	4	2	I	5	I	I	3	0			Max Wolf (1863 - 1032)
15	-	-			0	3	0 0	0	0	I	7	I	2	6	4	3	7	2	4	0	0	0			-	-	Quelle: Wikipedia

Importance of Galaxy Clusters

Ein merkwürdiger Haufen von Nebelflecken.

Es ist sofort zu sehen, wenn man die Tabelle oder die Tafel betrachtet, dass das Zusammendrängen der Nebel immer stärker wird, je weiter man in's Innere der Hauptinsel eindringt. Je näher man dem Puncte grösster Dichtigkeit kommt, umso dichter treten auch die Nebel an einander, so dass auf dem innersten Quadratgrad mehr als 320 einzelne Nebelflecken beisammen stehen. An der dichtesten Stelle dieses »Weltpoles« finden sich mehr als 70 Nebel auf der Fläche von 1/16 Quadratgrad.

Wir finden also hier ein völlig gesetzmässiges Verhalten in der Anordnung dieser fernen Welten; und dieser ungeheure Reichthum führt uns so eine Ordnung im Weltsystem vor Augen, die sicher für die Erkenntniss des Universums von allergrösster Bedeutung ist, von der wir uns aber auch zugestehen müssen, dass wir noch lange keine erschöpfende Erklärung für sie werden finden können.*)



And there is even something more!



> 1933: Clusters of galaxies: Dark Matter (Dynamics of the galaxies)

Multi-scale & physics problem!



The N-body problem:

The dynamics of stellar systems can be followed applying newton's law of gravity.

Arp 87 (NASA)

Messier 92 (INT)

j=N $\mathbf{F}_{i} = -\sum_{i=0, i\neq i}^{j=N} \frac{G m_{i} m_{j}}{r_{ij}^{2}} \,\hat{\mathbf{r}}_{ij}$ $j=0, j\neq i$

Coma (Dean Riwe, APOD)

First simulation by pen and paper



Evolution of the Universe



Setting the Framework



After two decades we can map the initial fluctuations of the structures in the universe with very high precission.

Setting the Framework

The growth of structures

10

Discretizing the matter distribution and starting from initial Gaussian density perturbation solving the N-body problem:

$$\mathbf{F}_{i} = -\sum_{j=0, j\neq i}^{j=N} \frac{G m_{i} m_{j}}{r_{ij}^{2}} \,\hat{\mathbf{r}}_{ij}$$

Speeding up the n² problem by building a Tree structure to approximate the forces.

The growth of Structures

⇒ formation of typical, cosmic structures like voids, filaments and collapsed objects (e.g. galaxies and galaxy clusters)

Active particles:

Speeding up the problem by individual time steps. Force needs to be calculated only for active particles.

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Speeding up the problem by individual time steps. Force needs to be calculated only for active particles.

Active particles:

Speeding up the problem by individual time steps. Force needs to be calculated only for active particles.

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Total active:

X bin= 5

73390182 47632510 121022692

0.00000245027

0.35

9.5%

overhead dominated

compute dominated

Particles to be distributed among MPI ranks:

Example: Gadget1

Large memory imbalance!

Example: Gadget2

> Perfect memory balance, but imperfect workload!

Example: Gadget3

Good balance (work/load) but communication overhead!

Speedup III: Tree-PM

 $\mathbf{\Phi}$ short

Splitting gravity in short range (Tree) and long range (FFT)

long

Domains are obtained by cutting the Peano-Hilbert curve into segments

$$\operatorname{mort}(\vec{x}) = -G\sum_{i} \frac{m_{i}}{\vec{r_{i}}}\operatorname{erfc}\left(\frac{\vec{r_{i}}}{2r_{s}}\right)$$

$$\Phi_{\vec{k}}^{\text{long}} = \Phi_{\vec{k}} \exp(-\vec{k}^2 r_s^2)$$

• density on the grid

 Φ^{s}

$$ho_m = rac{1}{h^3} \sum_i m_i W(ec{x}_i - ec{x}_m)$$

- solve for Φ using FFT methods $\Phi(\vec{x}) = \int g(\vec{x} - \vec{x}')\rho(\vec{x}')d\vec{x}'$
- calculate force using finite differences $f_{i,j,k}^{(x)} = -\frac{\Phi_{i+1,j,k} - \Phi_{i-1,j,k}}{2h}.$
- interpolate force back to particles

$$\vec{x}_i) = \sum_m W(\vec{x}_i - \vec{x}_m) \vec{f}_m$$

The growth of Structures

The distribution of galaxies in the universe and in simulations.

50 Mpc/h

How to treat the visible Universe:

Eulerian

discretized space

Lagrangian

discretized mass

kernel estimate

SPH

 $\langle A({f r})
angle = \int W({f r}-{f r}',h)\,A({f r}')\,{
m d}^3r'$

How to treat the visible Universe:

Now we can follow the equation of motion of two species of particle, but for the gas additional terms appear.

How to treat the baryons:

How to treat the baryons:

1 Mpc

2_dimensional velocity field a72 gas_nv at snap74 1.0 Mpc 0.6

Here, many details on the actual fluid properties go in.

Direct observation of Dark Matter:

How to get bigger ?

time

Dynamic range by computing power !

Growing computing power helps

Z3, 1941-1943 (Germany) 5 Computations per second

SuperMUC, 2013- (München) 3 Petaflops (3*10¹⁵ per second)

Moore's Law: Doubles all 1.5 Years

Z3 – SuperMUC:

1.4 Years

N-Body: 1970-2010: 1.3 Years

Hydro Simulations

Box2b/hr, Box0/mr

Extending scales to sub-grid

Dynamic range by subgrid models !

time

Sub-resolution star-formation:

Multi phase model (sub-scale)

Springel & Hernquist 2002

Star formation

supernova mass fraction

$$\frac{\mathrm{d}\rho_{\star}}{\mathrm{d}t} = (1-\beta)\frac{\rho_{c}}{t_{\star}}$$

star formation timescale

Cloud evaporation

Growth of cloud

$$\left. \frac{\mathrm{d}\rho_h}{\mathrm{d}t} \right|_{\mathrm{evap}} = A\beta \frac{\rho_c}{t_\star}$$

$$\frac{\mathrm{d}\rho_c}{\mathrm{d}t}\Big|_{\mathrm{TI}} = -\left.\frac{\mathrm{d}\rho_h}{\mathrm{d}t}\right|_{\mathrm{TI}} = \frac{\Lambda_{\mathrm{net}}(\rho_h, u_h)}{u_h - u_c}$$

Sub-resolution stellar evolution:

Stellar evolution model (sub-scale)

Energy: SNIa, SNIITornatore et al. 2003/2007star-formation rateMetals: SNIa, SNII, AGB winds
H,He,C,Ca,O,N,Ne,Mg
S,Si,Fe,Na,Al,Ar,NiTornatore et al. 2003/2007star-formation rate

$$R_{\rm SNIa}(t) = A \int_{M_{\rm B,inf}}^{M_{\rm B,sup}} \phi(m_{\rm B}) \int_{\mu_{\rm m}}^{\mu_{\rm M}} f(\mu) \,\psi(t - \tau_{m_2}) \,\mathrm{d}\mu \,\mathrm{d}m_{\rm B}$$

SNII and AGB rate: mass range of SN1a binary systems

(0.8-8Msol)

$$R_{\text{SNII}|\text{ILMS}}(t) = \phi(m(t)) \times \left(-\frac{\mathrm{d}m(t)}{\mathrm{d}t}\right)$$

Initial mass function (IMF):

Life-time: Maeder & Meynet 1989 Padovani & Matteucci 1993

Salpeter, Kroupa, Chabrier,

Arimoto & Yoshii

IMF:

Stellar yields: AGB: Groenewegen, Karakas SN1a: Thielemann SNII: Woosly & Weaver Romano, Kobayashi, ... $\phi(m) = dN/d\log m$

Life-time of stars

$$\pi(m) = \begin{cases} 10^{\left[(1.34 - \sqrt{1.79 - 0.22(7.76 - \log(m))})/0.11\right] - 9} & \text{for } m \le 6.6 \text{ M}_{\odot} \\ 1.2m^{-1.85} + 0.003 & \text{otherwise.} \end{cases}$$

Formation of galaxy clusters: gas

Formation of galaxy clusters: stars

Sub-resolution SMBH-formation:

Black Hole model (sub-scale)

Springel & Di Matteo 2006

Seeding

Constant seeding Seeding on m-sigma

Accretion on BH α-Bondi (Springl & Di Matteo 06) β-Bondi (Booth & Schaye 09) cold/hot (Bachmann et al. 14)

Feedback Thermal (Springel & Di Matteo 06) Bubbles (Sijacki et al. 07) Mass dependent (Steinborn 2015)

Merging Instant merging Based on velocity

....

....

Growth of Black Hole

$$\dot{M}_{
m B} = lpha imes \, 4\pi R_{
m B}^2 \,
ho \, c_s \simeq$$

 $\dot{M}_{ullet} = \min(\dot{M}_{\mathrm{B}}, \dot{M}_{\mathrm{Edd}})$

gas density

sound speed

 $4\pi \alpha G^2 M_{\bullet}^2 \rho$

 $(c_s^2 + v^2)^{3/2}$

Feedback by Black Holes $L_{\rm bol} = 0.1 imes \dot{M}_{ulletheta} c^2$ $\dot{E}_{\rm feedback} = f imes L_{\rm bol}$

efficiency

Positioning: Pinning to min. Potential Free floating

Merging galaxies with black holes

T = 0 Myr

10 kpc/h

http://wwwmpa.mpa-garching.mpg.de/gadget/right.html#Movies

Bigger: the challenge

Extending to the largest simulation currently possible, e.g. production runs on entire HPC systems !

STAN DOWN

General Constrains:

1) Fill significant fraction of memory with real particle/cell data instead of overhead !

80 bytes per Particle (MILLENNIUM XXL)

<mark>650 bytes per Particle</mark> (Magneticum)

=> 10⁷ per socket

Often still limiting factor in simulations which store full tree or cell structure (AMR) on every MPI task.

2) Formulate algorithm facing limitations in memory

Using buffers and checking their state major hassel for massive node parelelism (LOCKs !)

3) Formulate algorithm to be reproducable ?

Conserving order of operation is not always trivial, but make strongly non linear system difficult to compare (but this is almost a philosophical question) !

Interplay of different physics modules in Gadget3

find neighbors **Compute local Fill export list** contributions export list full? **Communicate list** APRIL PARTY I find neighbors **Compute** local **Fill return list** contributions all done? **Communicate results**

Tree-walk like, process all active particles

Gadget

Various physical proceses on various timescales ...

Sync-Point 35762, Time: 0.354961, Redshift: 1.81721, Systemstep: 5.56636e-06, Dloga: 1.56817e-05 Occupied timebins: non-cells cells dt cumulative A D avg-time cpu-frac 83736416883 0.008029050471 22.0% Х bin=20 88467428683 187287803634 < *712.64 6.8% X bin=19 4161559798 7573611723 0.004014525236 15083958068 * 219.80 X bin=18 689640843 1347123564 0.002007262618 63.43 3.9% 3348786547 * X bin=17 114047063 493679540 0.001003631309 1312022140 100.57 12.4% X bin=16 98886753 14.78 3.7% 424984562 0.000501815654 704295537 X bin=15 149882337 22957206 0.000250907827 180424222 24.04 11.9% X bin=14 1436369 5551598 0.000125453914 7584679 5.78 5.7% 6.8% X bin=13 10827 562559 0.000062726957 596712 3.46 X bin=12 22095 0.000031363478 23326 453 2.38 9.4% X bin=11 10 768 0.000015681739 778 2.20 17.4%

PM-Step. Total: 94008990945 93278812689

Sum: 187287803634

Time-steps

Simple Math: 0.5sec per step, 10 Million steps: 5.000.000 sec 1 day ~ 86.400 sec 1 week = 604.800 sec 1 month = 2.678.400 sec ⇒ 2 month to hanide 778 out of 1.7x10¹¹

Sync-Point 35762, Time: 0.354961, Redshift: 1.81721, Systemstep: 5.56636e-06, Dloga: 1.56817e-05 cumulative A D Occupied timebins: non-cells cells dt avg-time cpu-frac 83736416883 0.008029050471 712.64 22.0% Х bin=20 88467428683 187287803634 < *219.80 6.8% x bin=19 4161559798 7573611723 0.004014525236 15083958068 * bin=18 689640843 1347123564 0.002007262618 3348786547 63.43 3.9% х * X bin=17 114047063 493679540 0.001003631309 1312022140 100.57 12.4% X bin=16 98886753 0.000501815654 14.78 3.7% 424984562 704295537 X bin=15 149882337 22957206 0.000250907827 180424222 24.04 11.9% X bin=14 1436369 5551598 0.000125453914 7584679 5.78 5.7% X bin=13 10827 562559 0.000062726957 596712 3.46 6.8% X bin=12 22095 0.000031363478 23326 2.38 453 9.4% X bin=11 768 0.000015681739778 2.20 10 17.4%

PM-Step. Total: 94008990945 93278812689

Sum: 187287803634

Time-steps

What can be done ?

Avoid loops over all particles	
(but: drift, additional physics, additional nu	merics) the solver Molecular Network
Avoid almost empty All to All	
MPI_Alltoall(Send_count, 1, MPI_INT, Recv_ MYMPI_COMM_WORLD);	Count, ¹ 1, ² MPI_INT, <u>Tret-wak</u> Black Hole Feedback
for(j = 0; j < NTask; j++)	
Recv_count[j] = 0;	
MPI_Win_create(Recv_count, NTask * sizeo	f(MPI_INT), sizeof(MPI_INT),
MPI_INFO_NULL,MYMPI_CO	OMM_WORLD, &win);

MPI_Win_fence(0, win); for(j = 0; j < NTask; ++j)

if(Send_count[j] >.0) hift: 1.81721, Systemstep: 5.56636e-06, Dloga: 1.56817e-05 Sync-P MPI_Put(&Send_count[j], 1, MPI_INT, j, ThisTask, 1, MPI_INT, win);

Global time-step Level

Intermediate time-step Level

rac 22.0%

Tree-walk like, process all active particles

find neighbors

Compute local Fill export list

list

Fill return list

							·
х	bi <mark>n=19</mark>	MPI_WIN_fence	(U , WII);	0.004014525236	15083958068 *	219.80	6.8%
х	bi <mark>n=18</mark>	MPI_Win_free(&	&win);64	0.002007262618	3348786547 *	63.43	3 <mark>.9</mark> %
Х	bin=17	114047063 4	493679540	0.001003631309	1312022140	100.57	12.4 %
х	bin=16	424984562	98886753	0.000501815654	704295537	14.78	3.7%
х	bin=15	149882337	22957206	0.000250907827	180424222	24.04	11.9 %
х	bin=14	1436369	5551598	0.000125453914	7584679	5.78	5.7%
х	bin=13	10827	562559	0.000062726957	596712	3.46	6.8%
х	bin=12	453	22095	0.000031363478	23326	2.38	9.4 %
х	bin=11	10	768	0.000015681739	778	2.20	17.4%

Occupi

X

Sum: 187287803634

A must: MPI/OpenMP hybrid

Replacing MPI by OpenMP threads

For Gadget3 started 2012 with KONWHIR III project, but still ongoing effort ...

A must: MPI/OpenMP hybrid

value

Strong improvement for scaling

Actual scaling hydro computation

Scaling SuperMUC

Recent improvements ...

kCPUh

What we reached ...

2688 Mpc/h

M_dm = 1.9e6, M_gas =3.8e5 [Msol/h]

Largest Simulation (Box0/mr)

Setup: 2x4536³ = 186.659.085.312 particle Almost 20 times size of ILLUSTRIS or EAGLE **Full Physics + improved SPH:** 200 bytes per DM particle, 456 bytes per GAS particle **Complete SuperMUC Phase II:** 6 x 512 x 2 x 28 = 172032 tasks 1 MPI task per socket, 28 OpenMP per MPI 68.5 TB for single checkpointing reaching 170 Gbyte/sec, more than 3 Peta byte written **Dying nodes are the main hassle!** 12h longest contineous run, checkpoints all 1.5h

And the rest ...

very small volume / very high resolution

Physics:

cooling+sfr+winds Springel & Hernquist 2002/2003 Metals cooling Wiersma et al. 2009 SNIa,SNII,AGB Tornatore et al. 2003/2006

BH+AGN feedback Springel & Di Matteo 2006 Fabjan et al. 2010

Hirschmann et al. 2014 (std) Steinborn et al. 2015 (new)

HAR COMPARED

Thermal conduction 1/20th Spitzer

Dolag et al. 2004

Numerics: New Kernels: WC6 Dehnen et al. 2012

Low visc. scheme mr/hr (time dep. alpha)

Dolag et al. 2005 uhr (high order grad.) Beck et al. 2015

The many ways to form galaxies

https://www.youtube.com/watch?v=Je53JQhpTfk

Gyr = 0.28 z = 15.304

Conclusions

Cobe 1992

WMAP 2003

Improvements in computing facilities, code optimization and incorporating various important physical processes are helping to understand the universe throughout as well as the details on how galaxies and galaxy clusters are forming with time.

Magneticum/Box2/hr redshift=9.428 g=1.600 c=1.500 b=-0.000

https://www.youtube.com/watch?v=HHh_BcQ6fbQ

Distributing the Data

General concept of the Cosmosim Web Portal

Ragagnin et al, in prep

Testing indexing for file access

Cosmological Simulation Portal

c2papcososim1.srv.lrz.de

Ragagnin et al, in prep

Conclusions (II):

Direct dynamical range of 10⁶ almost reached Combination of optimization and growing computing power Further increased by "resonable" sub-scale models But need to be better validated and improved **Next simulations need new strategies** work distribution and massive vectorization (memory layout) First success across various scales **Global properties of Galaxy Clusters** AGN properties well reproduced in many respects **Diversity of CC and non CC clusters** Intra Cluster light and outskirts of Galaxies **Morphology of Galaxies Internal dynamics of Galaxies** Data federalization for hydro sims is challenging **Need complex infrastructure**