Using Supercomputers for PIC

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Outline

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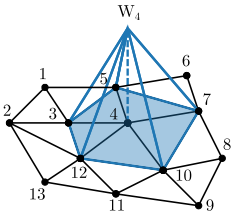
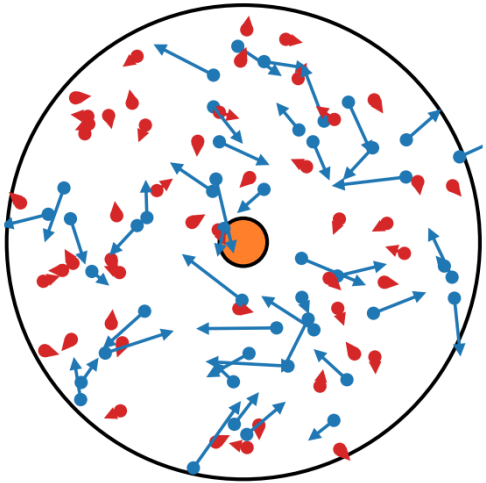
Recap: the Particle-In-Cell Method

PIC cycle:

1. Weight charge from particles to mesh
2. Solve Poisson equation ($\rho \rightarrow \mathbf{E}$)
3. Weigth field from mesh to particle
4. Move particles ($m\ddot{\mathbf{x}} = q\mathbf{E}$)





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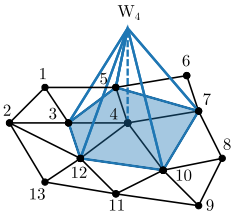

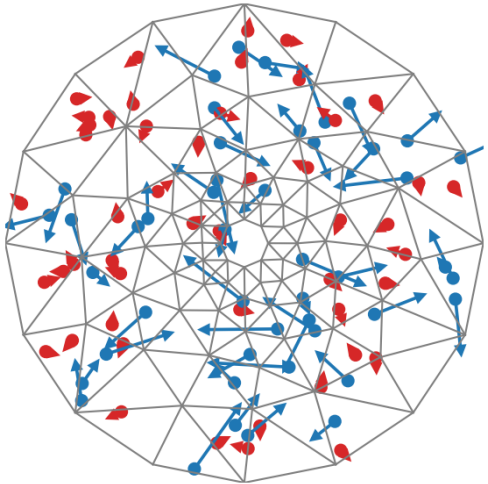

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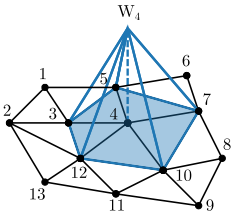

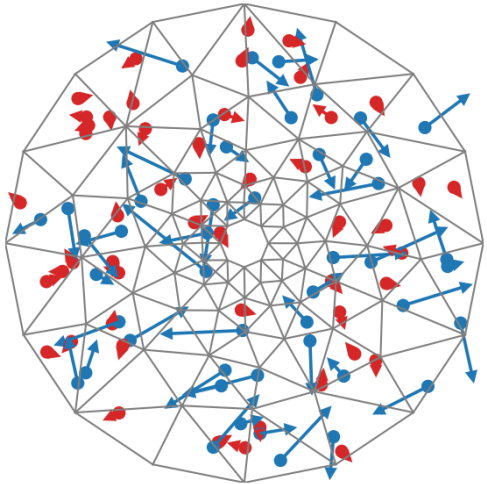

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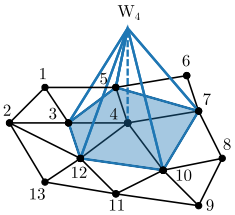

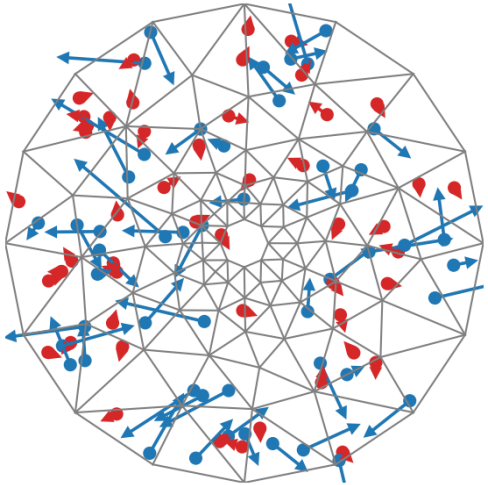

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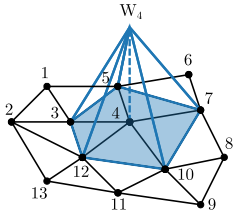

Recap: important criteria

Spatial (in Gmsh):

$h \lesssim 3\lambda_{De}$

$h \sim r/5$ (where r is radius of curvature)

Temporal (automatic in PTetra):

$\Delta t \ll \omega_{pe}^{-1} \quad (\Delta t < 1.62\omega_{pe}^{-1})$

$\Delta t \ll \omega_{ge}^{-1}$

$\Delta t < v_p^{-1} h$ for "most" particles p

$(\Delta t < kc^{-1} h$ for EM codes, for some $k)$

Birdsall and Langdon, *Plasma Physics via Computer Simulation*
Hockney and Eastwood, *Computer Simulation Using Particles*
Marholm, PhD thesis

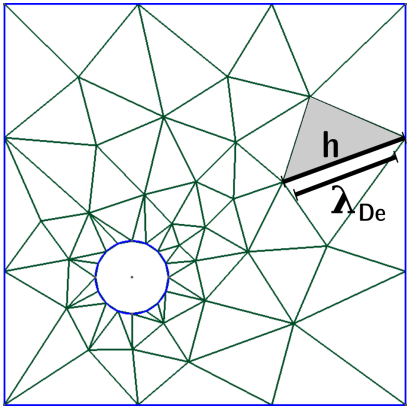

Figure: Illustration of cell diameter

Outline

Why supercomputers?

Larger simulations:
larger geometries, more particles

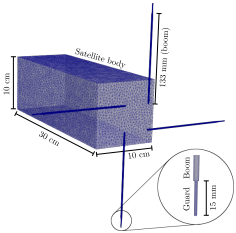

Figure: Large PTetra simulations of a CubeSat

Marholm, Marchand, *et al.*, DOI: 10.1109/TPS.2019.2915810

12 simulations $\times$ 16 cores $\times$ 8 weeks
$=$ 1536 core weeks (rough numbers)

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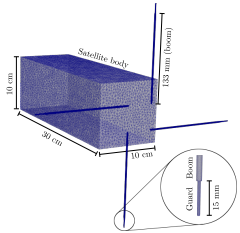

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More simulations:
embarrasingly parallel sweeps of parameters

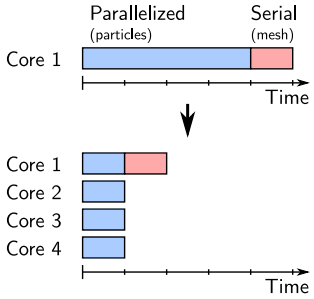
$\frac{e\Phi_p}{kT_e}$	r_p/λ_{De}				
	1.0	2.0	3.0	5.0	10.0
0	0.974	0.962	0.956	0.957	0.940
1	1.553	1.543	1.538	1.545	1.483
2	1.945	1.937	1.920	1.895	1.788
3	2.269	2.257	2.231	2.176	1.957
5	2.800	2.717	2.729	2.566	2.226
10	3.764	3.682	3.581	3.254	2.661
15	4.562	4.374	4.207	3.807	2.922
20	5.163	4.978	4.831	4.251	3.132
25	5.688	5.492	5.207	4.520	3.325

Figure: 45 of 594 small PUNC++ simulations of probes Darian, Marholm, *et al.*, DOI: 10.1088/1361-6587/ab27ff

594 simulations $\times$ 1 core $\times$ 1 week
$=$ 594 core weeks (rough numbers)

Outline

Parallel programming



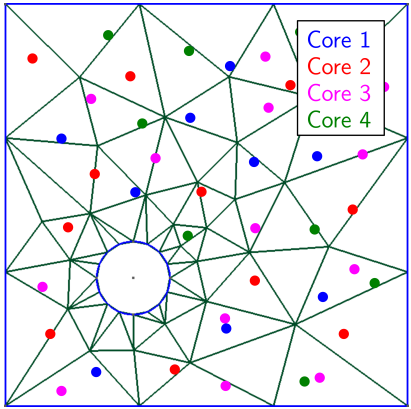


Figure: Different particles handled by different cores

Example of parallelized mesh part

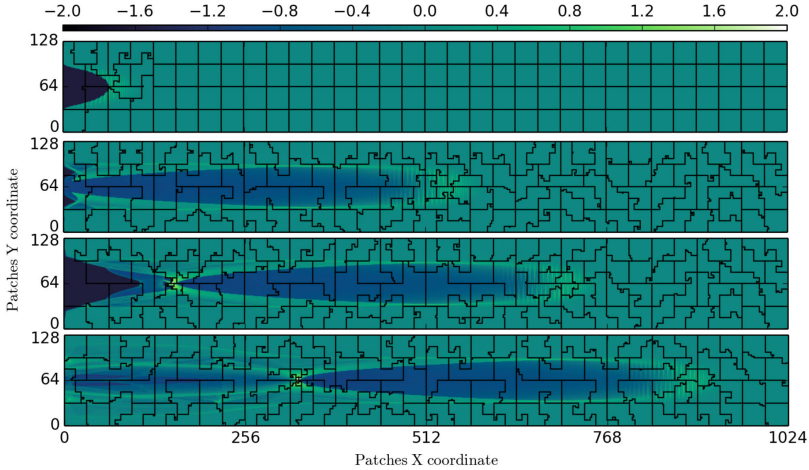
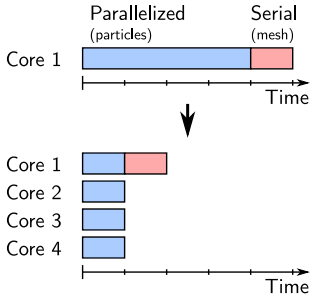


Figure: Load balancing in SmileiPIC `https://smileipic.github.io/Smilei/highlights.html`

Parallel programming



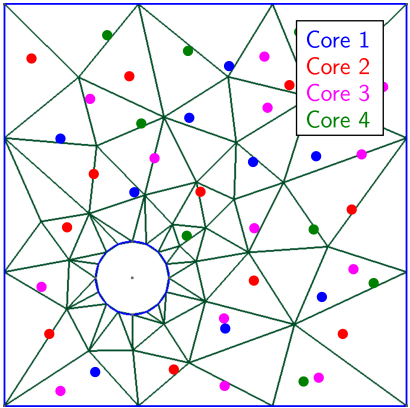
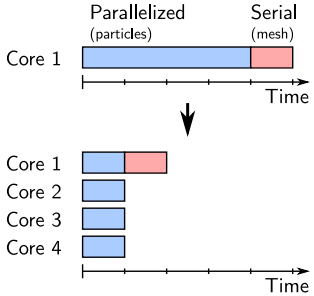


Figure: Different particles handled by different cores

Amdahl's law



$$\text{Speedup} = \frac{N}{(1-p)N + p}$$

p – Parallelized fraction
N – Number of processes

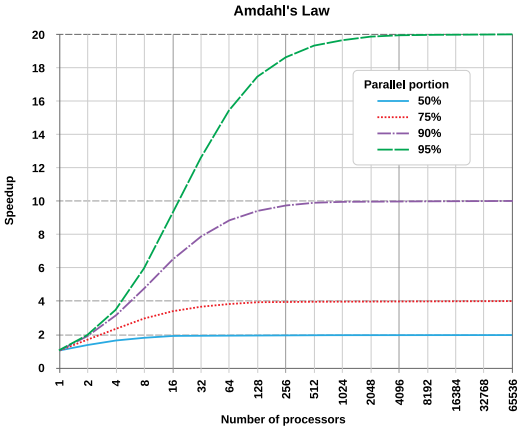
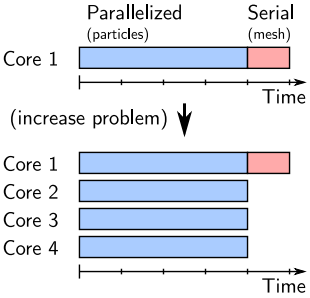


Figure: From Wikipedia

Gustafson's law



$$\text{Speedup} = (1 - p) + pN$$

p – Parallelized fraction
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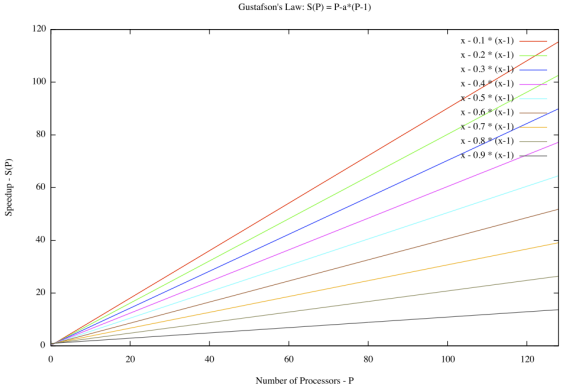


Figure: From Wikipedia

Strong and weak scaling

Strong scaling:

- Fixed problem size (Amdahl)
- Faster with more cores

Weak scaling:

- Fixed size per core (Gustafson)
- Similar execution time with more cores

Example: OSIRIS – Cartesian PIC code
10^{10} cells, 10^{13} particles, ~ 2 PFlop/s

Fonseca *et al.*, PPCF 55 (2013)

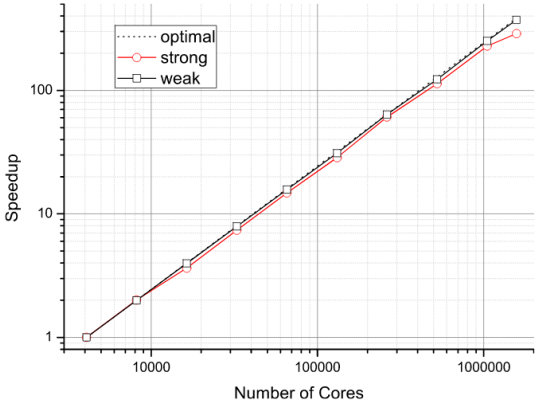
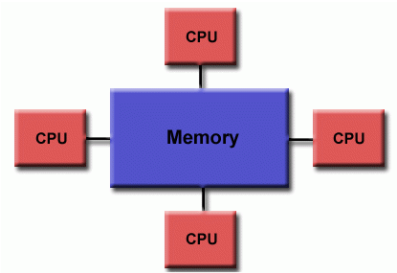


Figure: Scaling of OSIRIS (2013)

Memory architectures

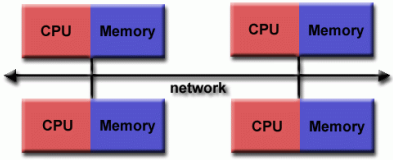
Shared memory (multicore PC, GPU):



Every core can read/write to all the memory. Must synchronize.

- OpenMP for CPUs
- OpenCL/CUDA for GPUs

Distributed memory:



Every core has it's own memory, and the cores must send each other data.

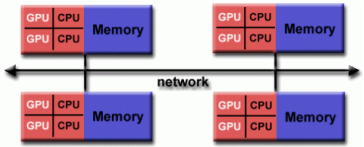
- Message Passing Interface (MPI)

https://hpc.llnl.gov/documentation/tutorials/introduction-parallel-computing-tutorial

Outline

Supercomputers

Supercomputer =
many computers (nodes) + fast network



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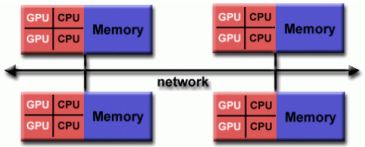

Typical storage of a particle:

x	y	z	v_x	v_y	v_z	q	m

x	y	z	v_x	v_y	v_z	w

7 doubles $\times$ 8 bytes = 56 bytes

Standard node at Saga:

192 GB RAM, 40 cores
$\Rightarrow$ 4.8 GB $\approx$ 4 GB RAM/core
$\Rightarrow$ upper limit: 75 mill. particles/core (all species)
minus storage required for mesh solver

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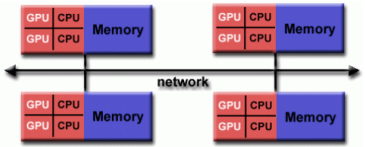

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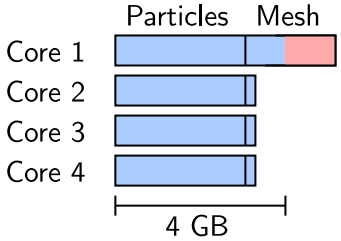

Usually okay if cores on same node

Supercomputers

	My laptop	Saga	Fugaku
CPU cores	2		
RAM [GB]	32		
GPUs	0		
Nodes	1		
TFlop/s	∼0.05		

Top500 List November 2021
https://www.r-ccs.riken.jp/en/fugaku
https://documentation.sigma2.no/hpc_machines/saga.html

Supercomputers

	My laptop	Saga	Fugaku
CPU cores	2	16 064	
RAM [GB]	32	99 840	
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Supercomputers

	My laptop	Saga	Fugaku
CPU cores	2	16 064	7 630 848
RAM [GB]	32	99 840	5 087 232
GPUs	0	32	0*
Nodes	1	364	158 976
TFlop/s	∼0.05	795	537 212

*somewhat unusual. Summit has 27 648.

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Logging in with SSH

Basic login with SSH

```
$ ssh <username>@<host>
```

Example

```
$ ssh sigvaldm@saga.sigma2.no
```

We use Saga as example (requires user). Similar elsewhere.
HPC facilities usually have good docs. Read them.

Authenticating with keys instead of password

Create a private/public key-pair

```
$ mkdir -p ~/.ssh # Only necessary if folder does not exist
$ cd ~/.ssh
$ ssh-keygen -t rsa -b 4096 -f saga # 4096 bit RSA encryption
...
$ ls -l saga*
-rw------- 1 sigvald sigvald 3369 Jan 31 11:41 saga         # Private
-rw-r--r-- 1 sigvald sigvald  737 Jan 31 11:41 saga.pub     # Public
```

Make sure the private key (`saga`) has permissions `-rw-------`. If not, run `chmod 600 saga`.

Careful! "No passphrase" is convenient, but then you must make sure private key can not be stolen (do not store on servers, etc.). See also `ssh-add`.

Authenticating with keys instead of password

Remote machine you're logging into need the public key.
Copy contents of `~/.ssh/saga.pub` to a new line in `~/.ssh/authorized_keys` on remote.

One-liner that copies public key to remote

```
$ cat ~/.ssh/saga.pub | ssh <username>@saga.sigma2.no "mkdir -p ~/.ssh && cat >> ~/.ssh/authorized_keys"
```

Login with key

```
$ ssh -i ~/.ssh/saga <username>@saga.sigma2.no
```

`-i ~/.ssh/saga` can be omitted if key has default name (`id_rsa`)

Create alias for convenience

Add the following lines to ~/.ssh/config to create alias

```
Host saga
    HostName saga.sigma2.no
    IdentityFile ~/.ssh/saga
    User <username>
```

Login with alias

```
$ ssh saga
```

Similar for GitHub, etc.:
Upload public key on `github.com` → Settings → SSH and GPG keys → Add SSH key
Make sure you're connecting to GitHub via SSH and not HTTP.

Outline

Transferring files with rsync

Rsync synopsis

```
$ rsync <options> <source> <destination>
```

Example: transfer Geometry folder to MyProjects folder on Saga

```
$ rsync -aP Geometry saga:Projects
```

Example: transfer it back

```
$ rsync -aP saga:Projects/Geometry .
```

Unlike SCP, rsync continues on interrupted files next time.

Transferring files via mounted directory

Mount a remote directory to a local one

```
$ mkdir ProjectsOnSaga # Only necessary the first time
$ sshfs saga:Projects ProjectsOnSaga
```

Use `ProjectsOnSaga` like any other folder.

Unmount when done

```
$ umount ProjectsOnSaga
```

Outline

Job scripts (Slurm)

run.sh (inside simulation folder)

```
#!/bin/bash

#SBATCH --job-name=sph1V      # Name for your reference
#SBATCH --account=nn9299k     # Where to charge the core hours
#SBATCH --time=24:00:00       # Max wall-clock time. Set mpitimemax in pictetra.dat one hour less.
#SBATCH --ntasks=4            # Number of cores
#SBATCH --mem-per-cpu=3920M   # Memory per core

set -o errexit # Exit the script on any error
set -o nounset # Treat any unset variables as an error

# Make sure to load dependencies (e.g. gfortran and MPI) using the module system
module purge
module load foss/2020a

# Run PTetra using MPI, and store output
mpirun ./mptetra > mptetra.log
```

Job scripts (Slurm)

To allocate entire nodes

```
# #SBATCH --ntasks=4          # Removed
#SBATCH --nnodes=1            # Number of nodes
#SBATCH --ntasks-per-node=4   # Number of cores per node
```

Running on multiple cores on a workstation

```
$ mpirun -n 4 mpitetra | tee mptetra.log
```

Outline

Managing jobs (Slurm)

Submit job

```
$ sbatch run.sh
```

Inspect queue

```
$ squeue -u <username>
```

Cancel job

```
$ scancel <job number>
$ scancel -n <job name>
```

For other workload managers: `https://slurm.schedmd.com/rosetta.pdf`

Managing jobs

Inspect quotas (Sigma2-specific)

```
$ cost --detail # core hours
$ dusage        # disk usage
```

Inspect PTetra output

```
$ tail -f mptetra.log
```

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