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VITAE: VIrTual brAin pErfusion

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de Toulouse



VITAE

VirTual brAin pErfusion

ERC Proof of Concept VITAE (GA 825829)

JCAD 2020

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Contributors: Jean-Daniel Julien, Maxime Berg, Myriam Peyrounette, Pierre Elyakime, Yohan Davit, Maxime Pigou ,
Sylvie Lorthois

Outline

Context

Software

Benchmarks & results

Return on experience

Perspectives

Context

Problem

Blood flow is vital for feeding and cleansing neurons

Recent discovery

Blood flow decrease before measurable cognitive decline in Alzheimer's Disease (2016)

Novel therapeutic strategy

development of drugs targeting the vascular system

Idea

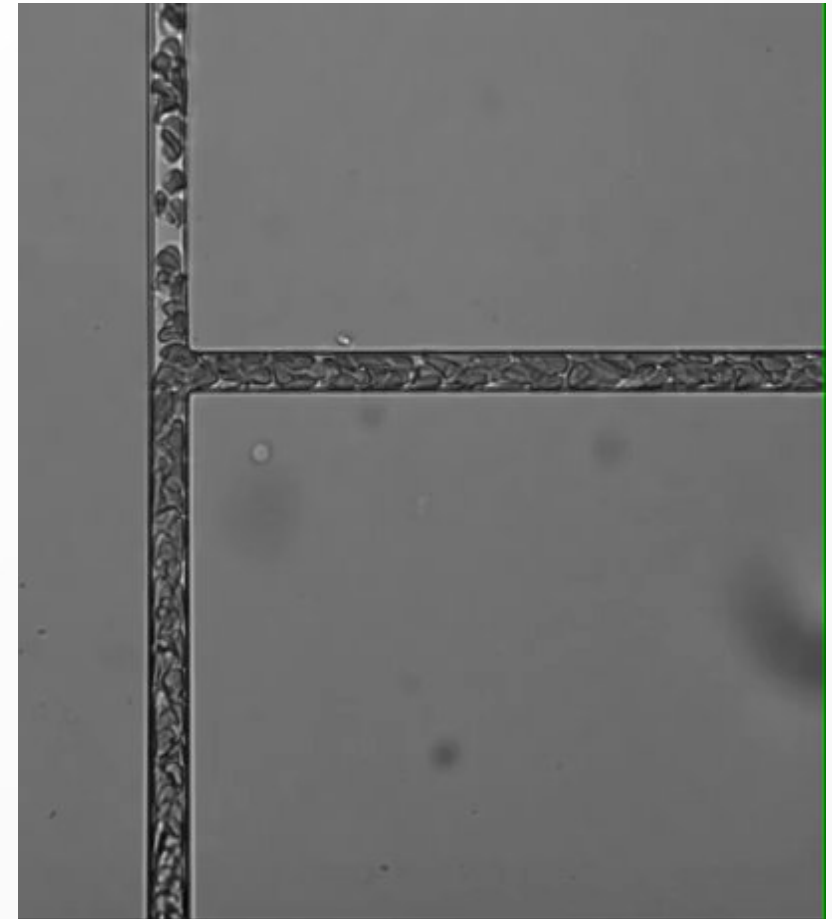
Use HPC simulation of cerebral blood flow to accelerate vascular targeted drug development

Background

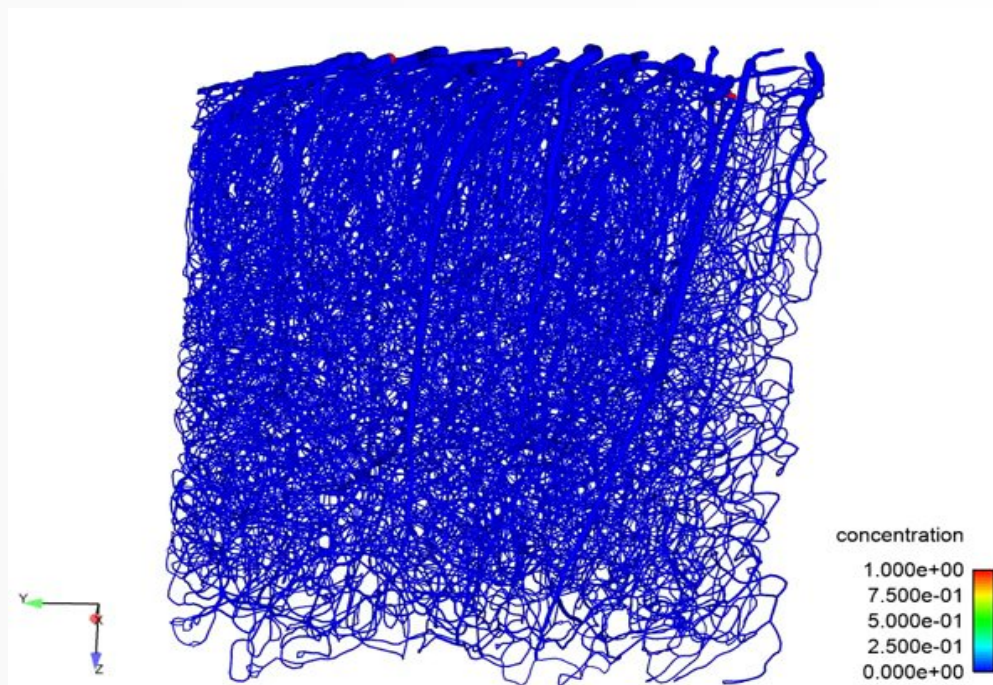


Blood flow study

- Vascular networks have a complex topology
- Blood itself is a complex fluid



Blood flow simulations



PhD IMFT Maxime Berg, Berg et al. 2020

1 mm³ mouse brain

Previous Simulations (using V1.0)
14k vessels

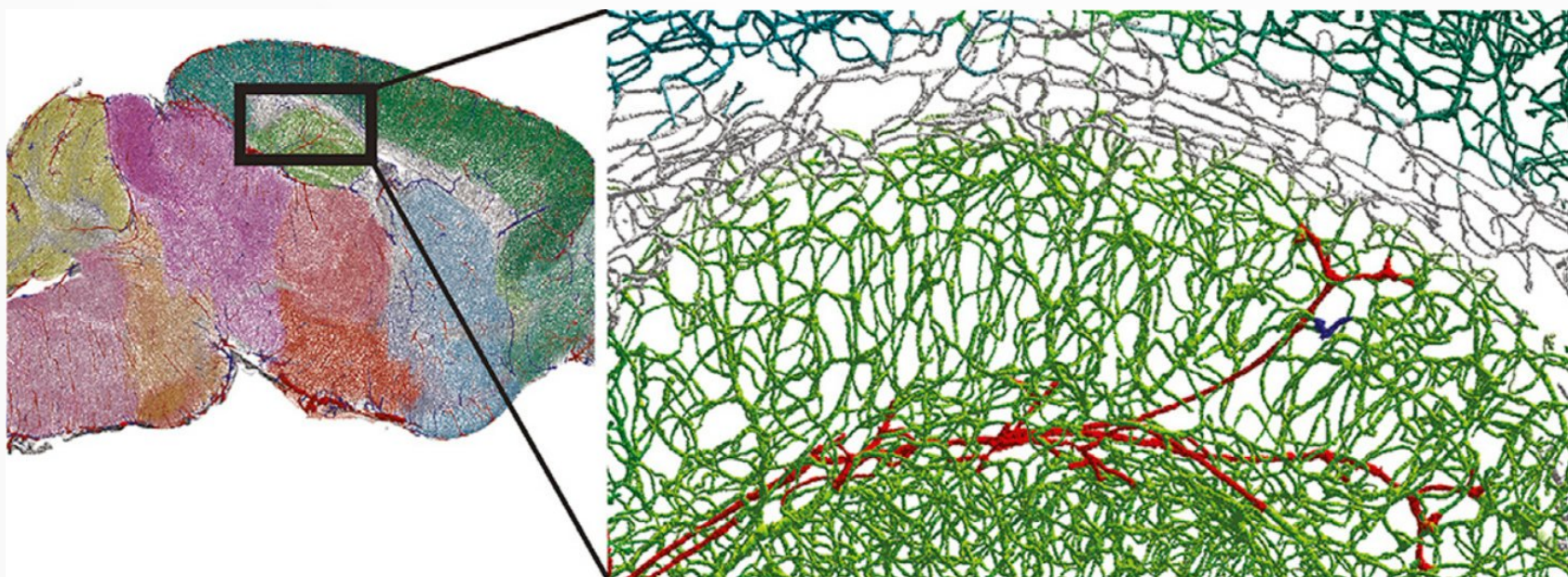
Issue

Does not scale up for
large vascular networks

Whole mouse brain imaging

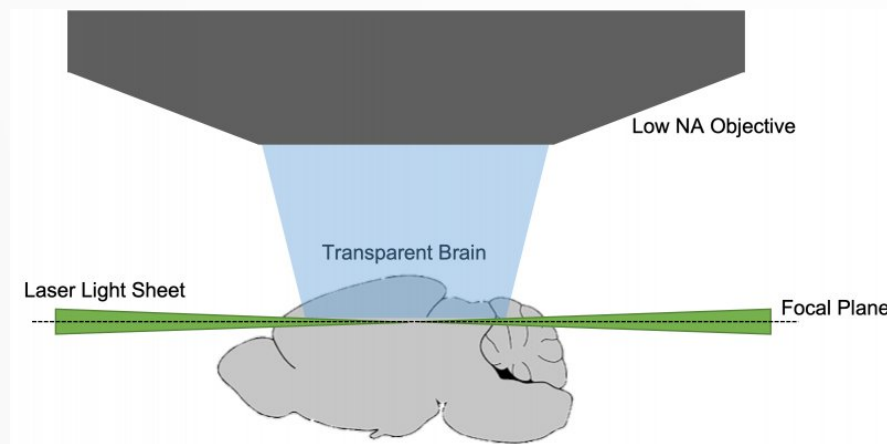
International effort to acquire whole mouse brain vascular networks

2020: publication of a pipeline reconstructing the full vascular network of a mouse brain at *Institut du Cerveau et de la Moelle épinière (ICM)*

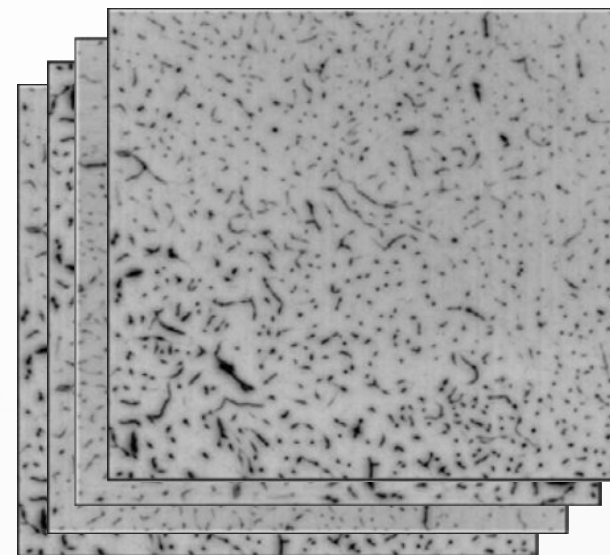


Whole mouse brain imaging

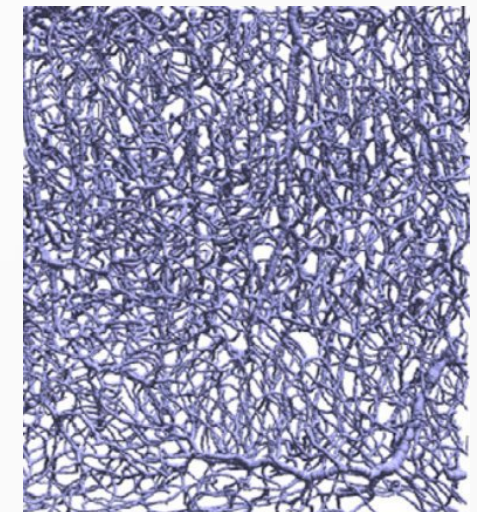
Example: Lightsheet microscopy



visikol.com



Kirst et al. 2020

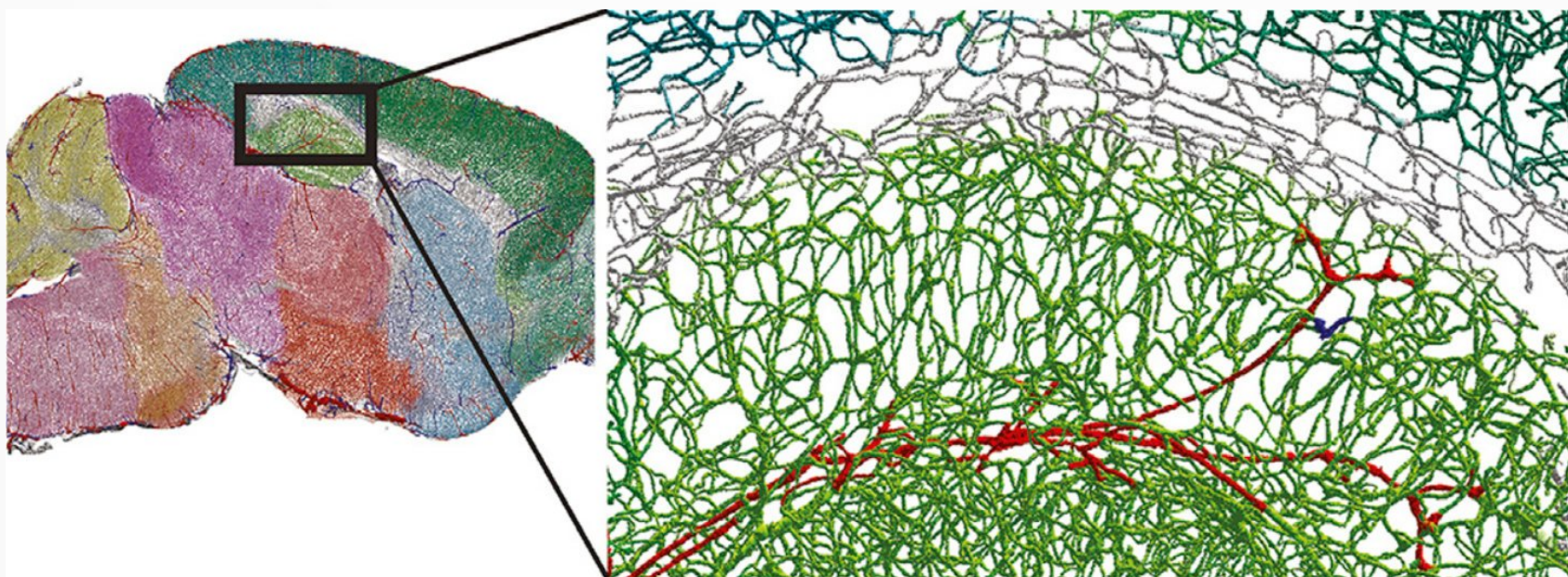


Kirst et al, 2020

Whole mouse brain imaging

Simulation goals :

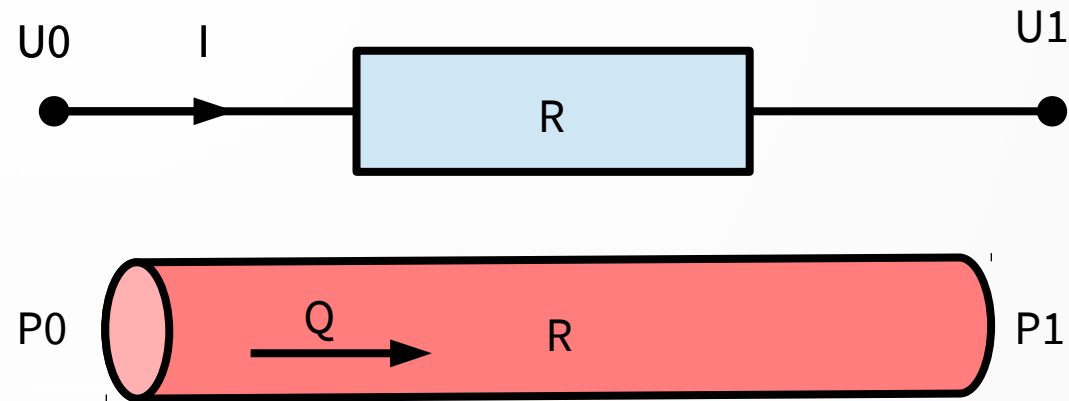
- 5M to 10M vessels
- Pressure and blood flow
- Distribution of red blood cells
- Nutrient and drug delivery



Flow solving

Electrical analogy

- $\Delta U = RI$
- $\Delta P = RQ$



Matrix formulation for full brain

- Inversion of a $\sim 5M \times 5M$ sparse square matrix M
- Requires gradient descent like algorithm
- Requires parallel calculation

$$Mp = y$$

History

- 2014: V1 start
 - Research code in C++
 - Not scalable
 - Completely written on top of *PETSc*
- 2018: ERC POC grant
 - Scaling for full brain
 - Code industrialization
- 2019: V2 start
 - Hiring dedicated software engineer
 - Codebase mostly rewritten
- 2020: first tests on full brain data (Kirst et al.)

The VITAE software

Design goals

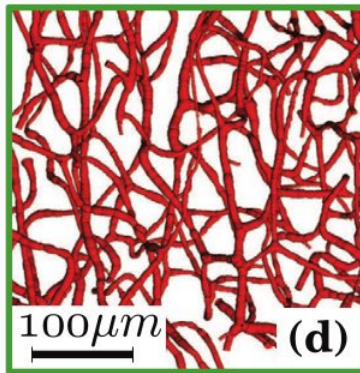
- Fully parallel processing
- CPU efficient
- Modern C++
- Modular API
- User friendly
- Fully documented

Dependencies

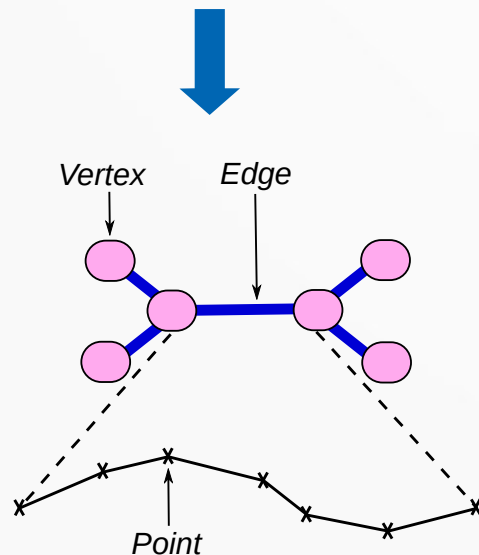
- std=c++14 (gcc9, ICC 18 & 19)
- Compilation (cmake-3.10)
- MPI (OpenMPI-2.1.1, MPICH-3.3.2)
- Parallel IO (HDF5-1.10.5)
- Linear algebra (PETSc-3.7.7)
- Graph partitioning (Parmetis-4.0.3)
- JSON Config (nlohman-json-3.7)
- JSON Schema #7 (pboettch-2.0)
- Unit tests (cxxtest-4.4)

Data model

Vascular networks have a graph structure



Peyrounette et al. 2018

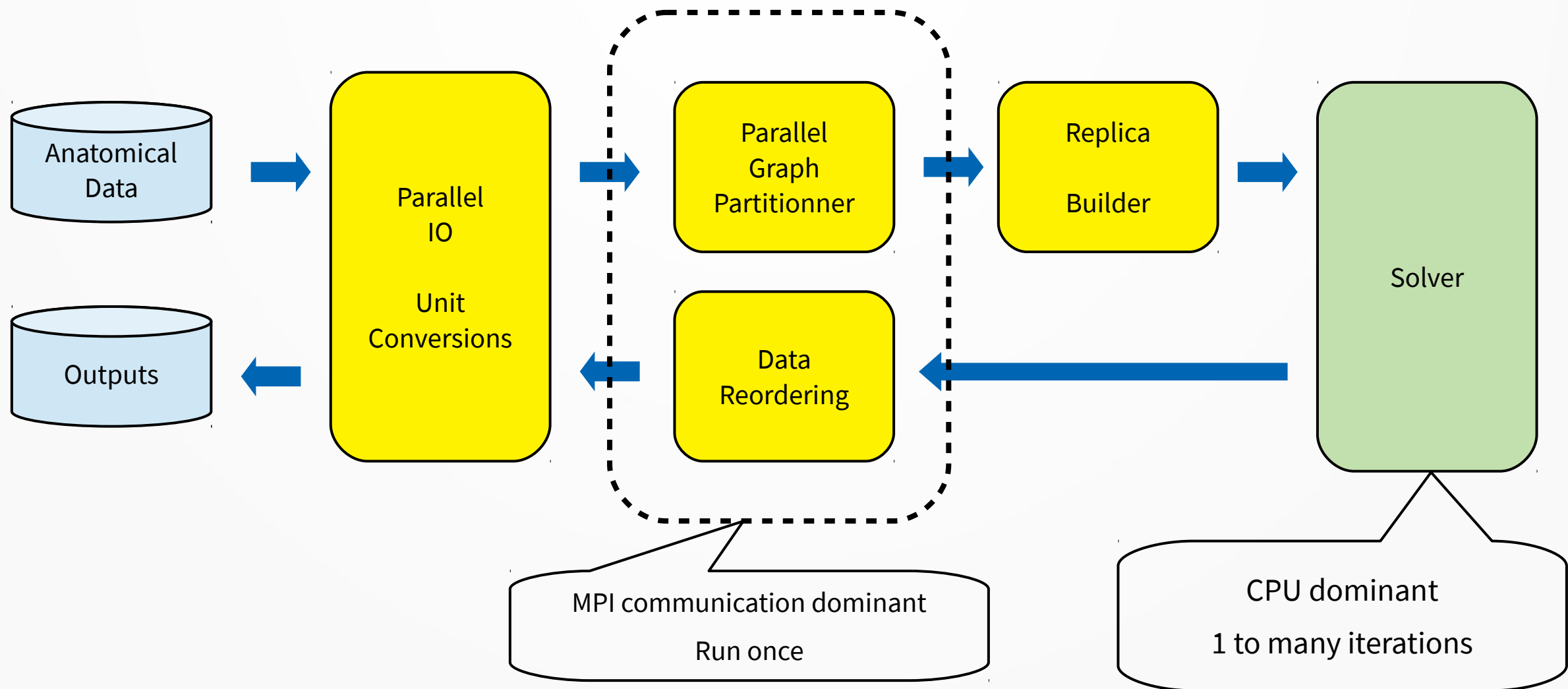


Three major categories

- vertex for bifurcations
- edge for vessels
- point for vessels path (grouped by edge)

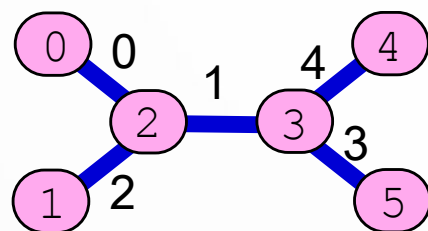
Network	Size [vertex]	Memory footprint estimation
[V1] Kleinfeld (mouse)	10 k	11.7 MiB
[V2] Average mouse brain	5 M	6.1 GiB
Average Human brain	> 1 G	> 1.2 TiB

Data flow

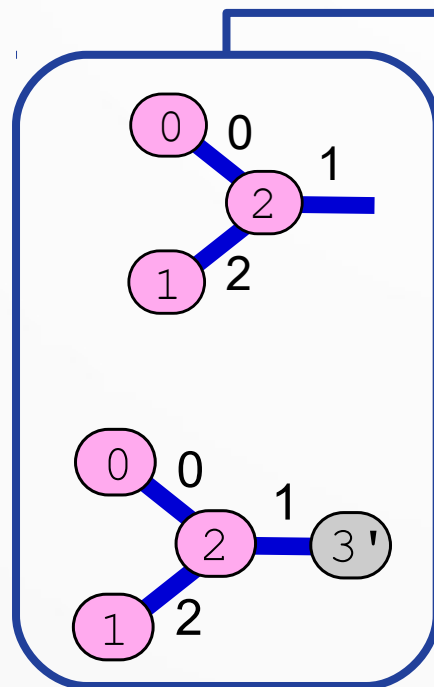


Graph Partitioning

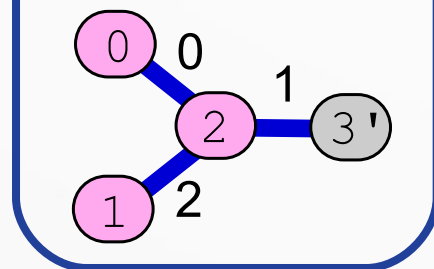
Initial graph



Partitioning
minimize nb of edge cuts



Replica insertion
(ghosts)

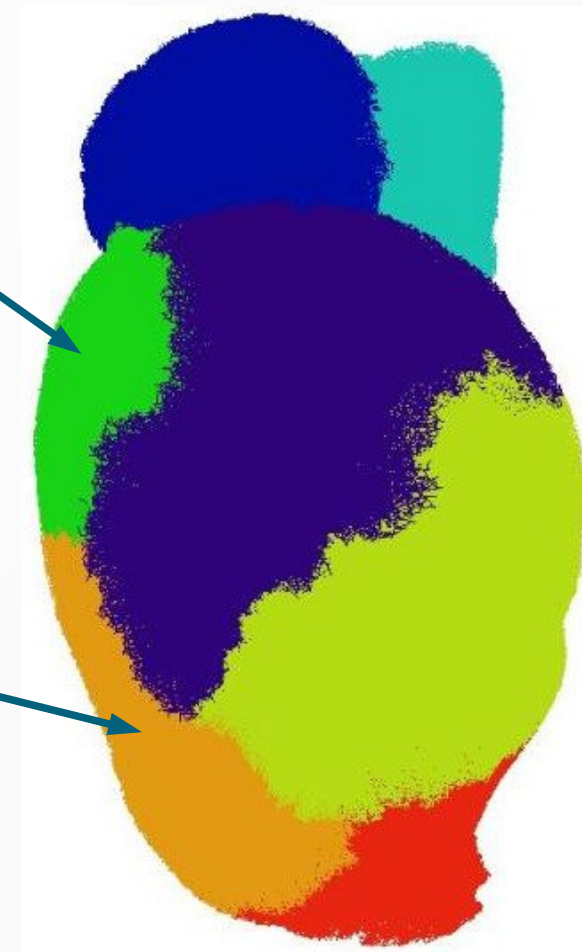


process0

process1

...

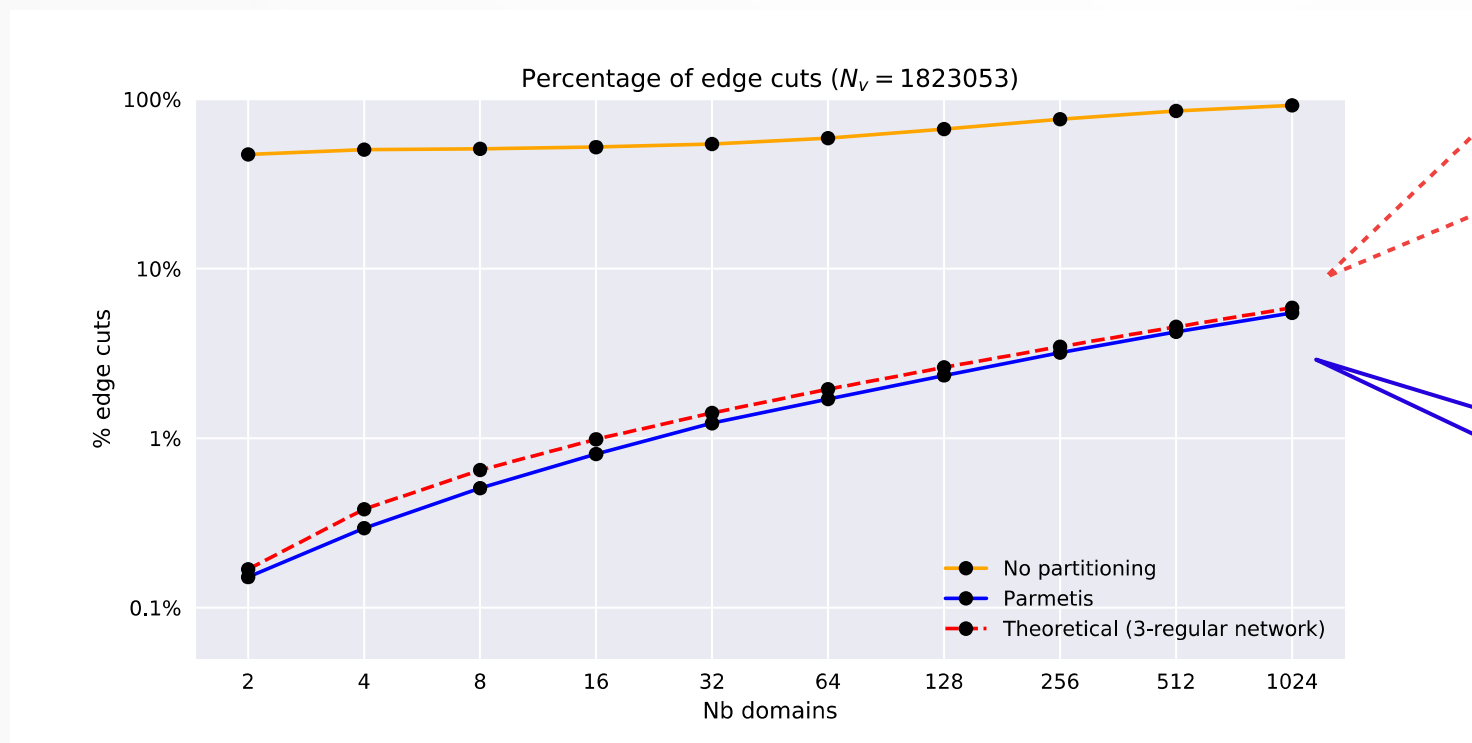
8 partitions
(Parmetis)



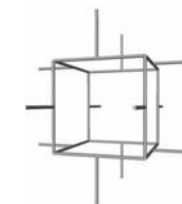
PhD Marion Giraud IMFT

Benchmarks

Efficiency of graph partitioning



Lower is better



3-regular
Synthetic network

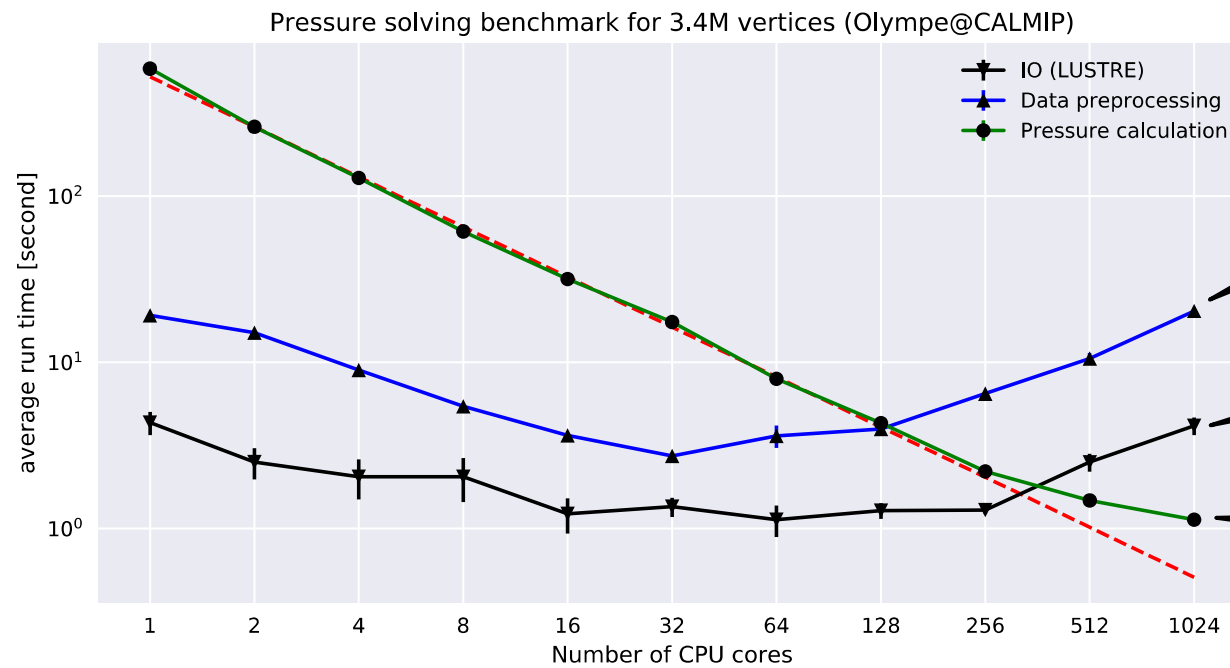
$$ncut \sim O(N_d^{1/3} \times N_v^{2/3})$$



1.8M vertex network
(Kirst 2020 CU)

Benchmarks

MPI CPU scaling for Flow Solver



Partitioning
and pre/post processing
MPI communication dominant
run once

File system access
run once

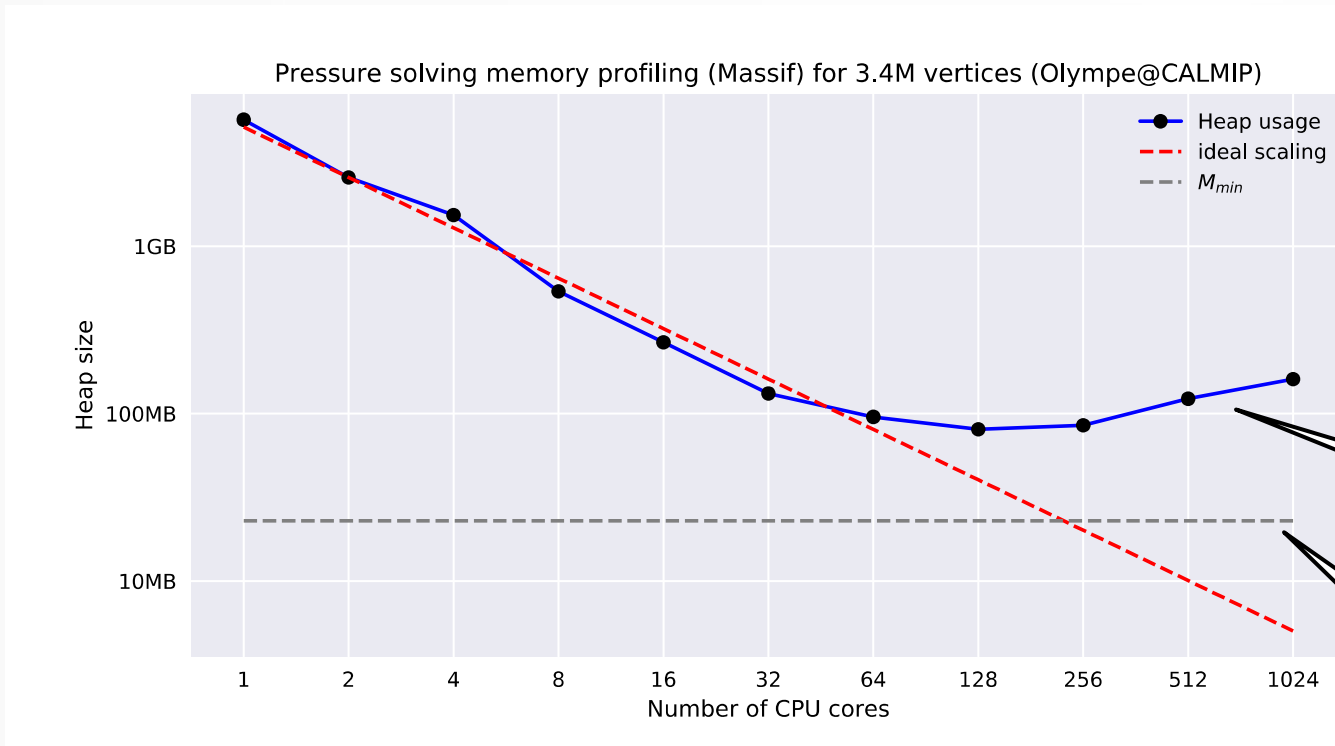
Flow calculation
CPU dominated
run many

Lower is better

Benchmarks

MPI peak memory scaling for 1 process

Profiling tool: `valgrind --tool=massif`



Lower is better



`ms_print massif.out`

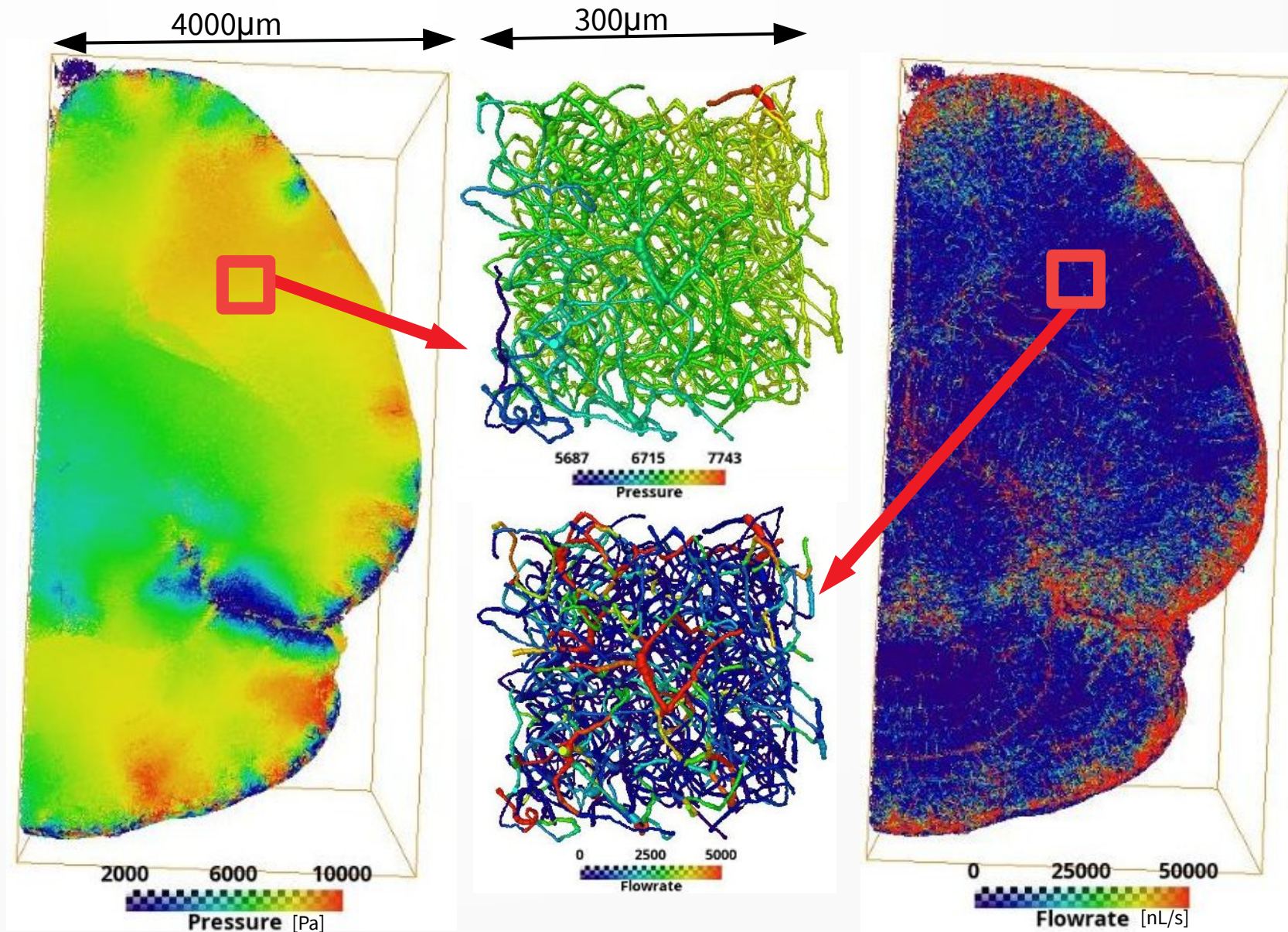
Memory excess
Dominated by
Parmetis MPI buffers

*Minimum
Process size*

Results

Full brain pressure and flow rate calculation

- Half mouse brain
- Data source:
 - ICM (Kirst et al. 2020 CU)
 - HDF5 File size: 507MB
 - Nb vertices: 3.4M
 - Nb edges: 4.7M
- Calculation
 - Olympe@CALMIP
 - ~10 minutes
 - one process
- Visualization
 - Avizo



Issues

Technical

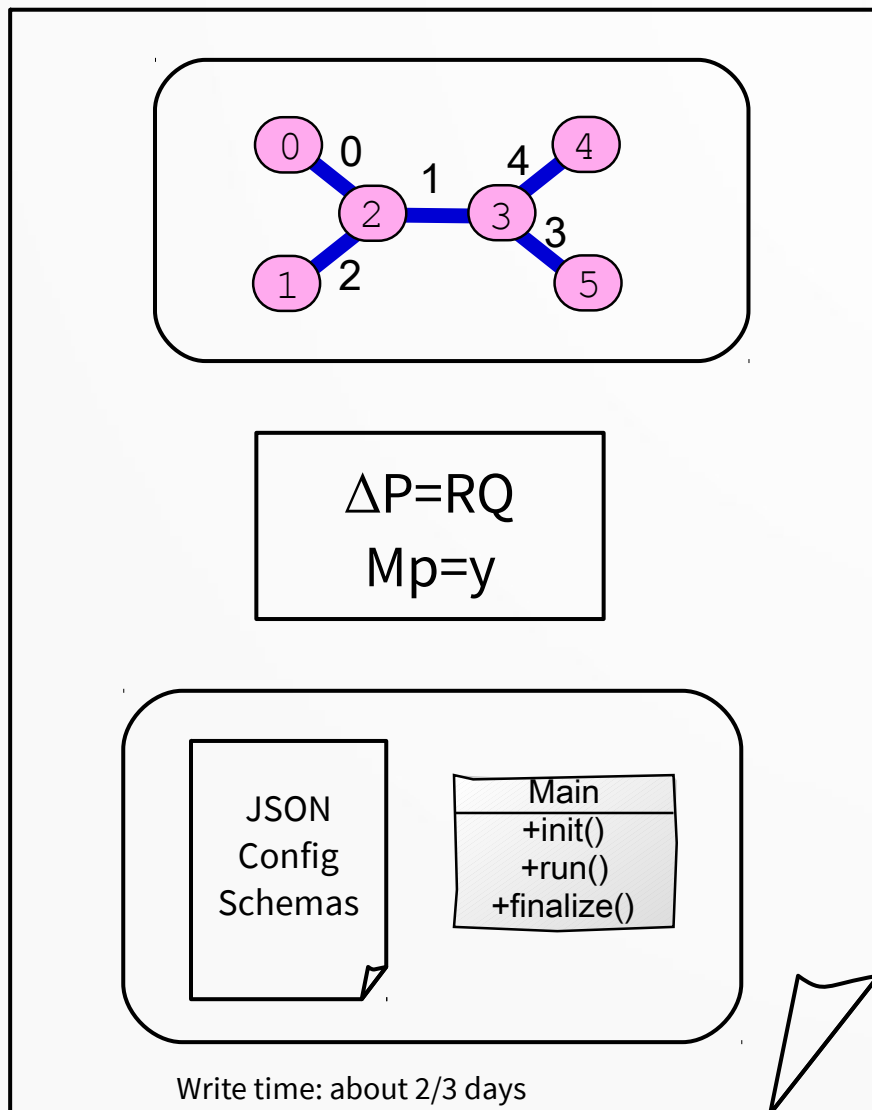
- PETSC installation & config
- Direct use of HDF5 instead of PETSc wrapping
- MPI is not very well suited for graph manipulation
 - Graph structure requires to call various mixtures of `Mpi_Alltoall()` and `Mpi_Alltoallv()`
 - Average nb of connected domains is 13 which may require specific optimizations
- Intel ICC18 compiler (`std::shared_ptr<std::array>`, etc.), ICC19 easier
- CMake steep learning curve, one has to use modern version
- C++ version of dependencies often not available or incomplete
Example: HDF5, PETSc, MPI, etc.

Other

- Semantic
 - Example: disambiguate UIDs versus global offset and local offset

Solver teamwork

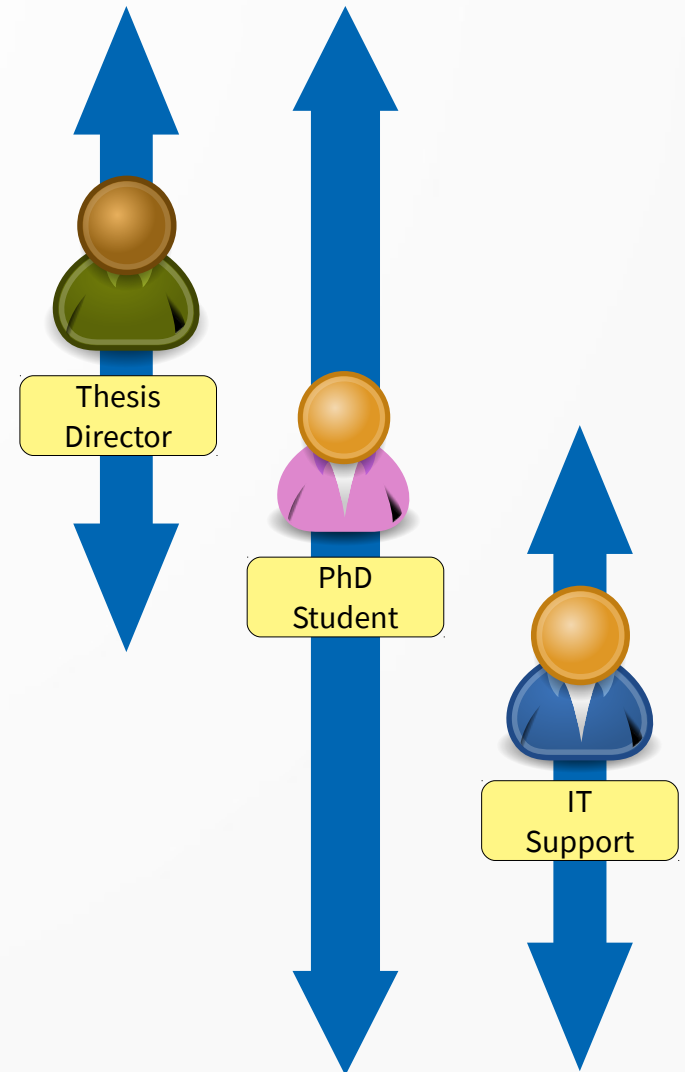
Solver specifications



1) Scientific goal
Mesh definition

2) Numerical scheme
Algorithm

3) Code Specifications
Data, Object Model



Software quality

Continuous integration

- Git versionning
- Wiki
- Runners
- unit tests



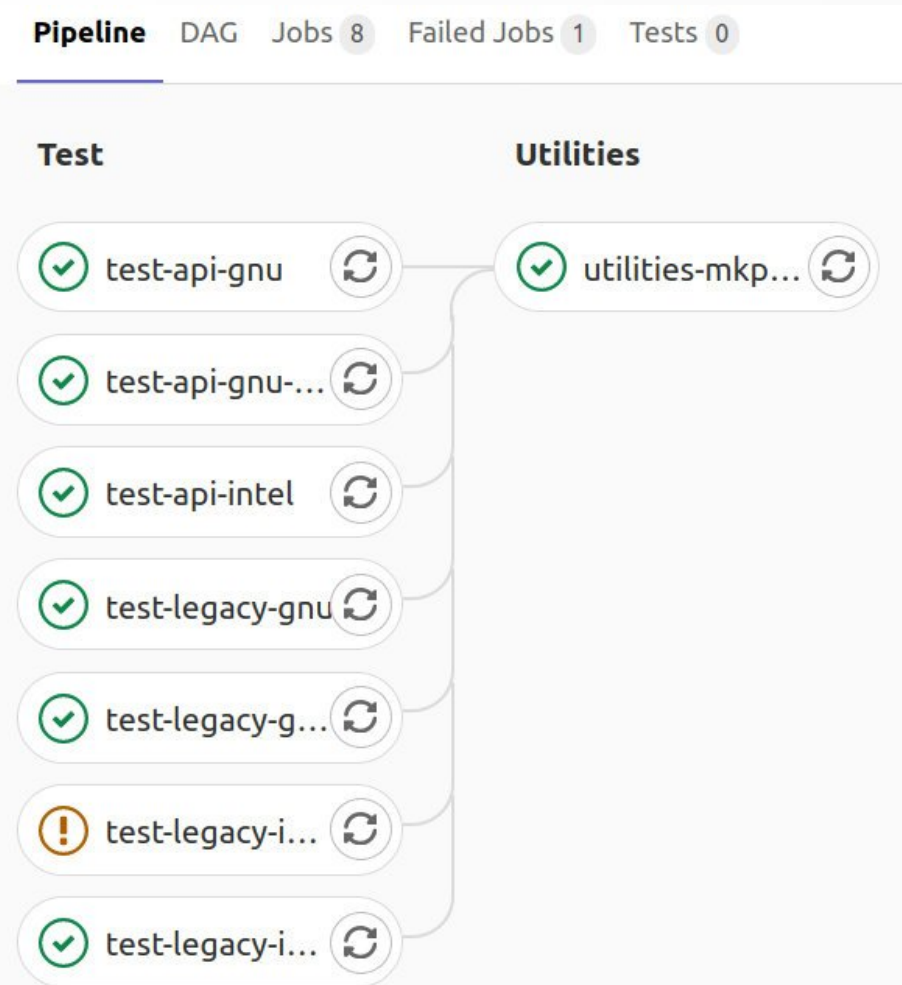
GitLab

Naming convention document

Schema validation

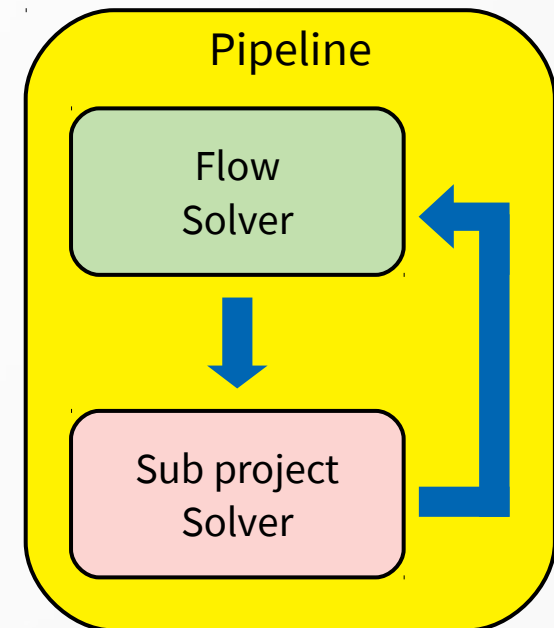
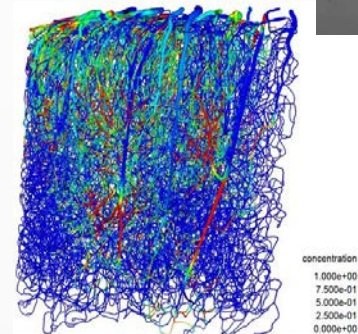
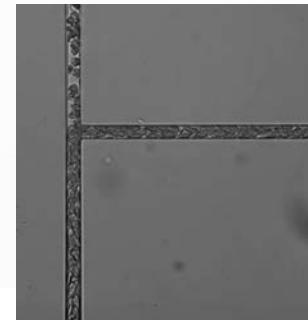
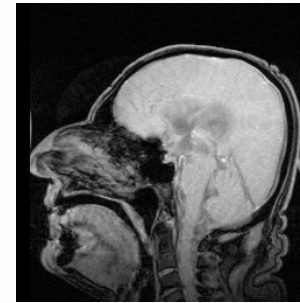
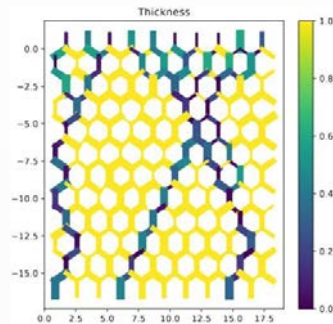
Documentation

- Latex manual
- Rich doxygen code snippets



Scheduled Projects

- Solver: *BrainPulse*
 - Solver for blood pulsatility
 - Project lead: Alexandra VALLET (univ. oslo)
- Solver: *BioGrow*
 - Simulation of bacterial growth
 - Project lead: Jean-Daniel Julien
- Solver: *PhaseSeparation*
 - Calculation of blood cells concentration in plasma
 - Initial author: Maxime Berg
 - Porting to VITAE API V2: Maxime Pigou
- Solver: *MassTransport*
 - Simulation of solute transport into blood
 - Initial author: Maxime Berg
 - Porting to VITAE API V2: Alexandre Sauv 



depth 2
iterative solvers

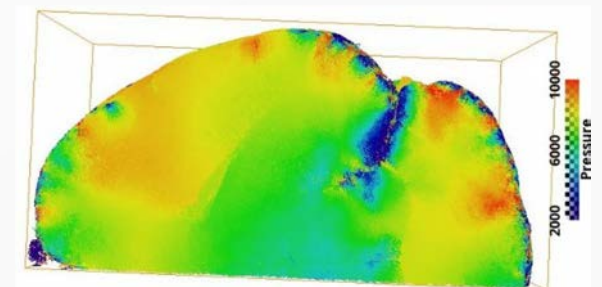
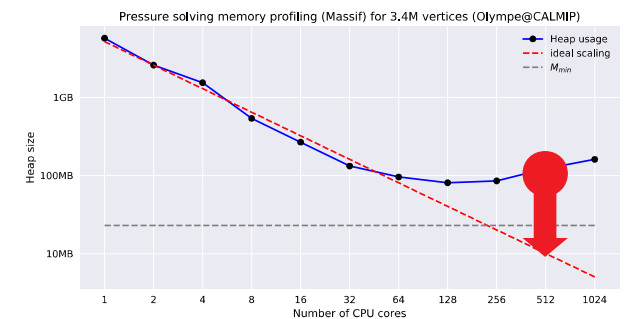
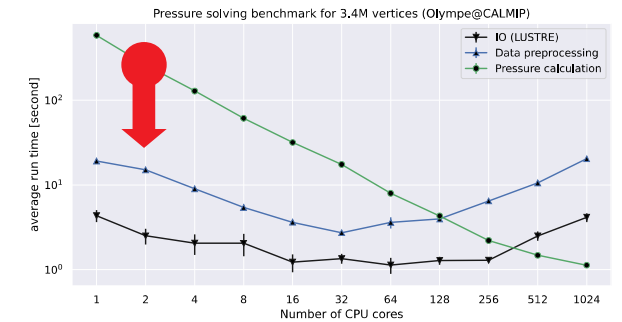
Evolutions

Technical

- Improve flow solver convergency time (*PETSc* KSP methods)
- Improve partitioning scaling (Example: test *PT-SCOTCH*)

Data exploitation

- New vascular networks from various collaborations
- Reduction of full brain results



Questions

