Challenges in 3-D simulation of vascular graph remodelling

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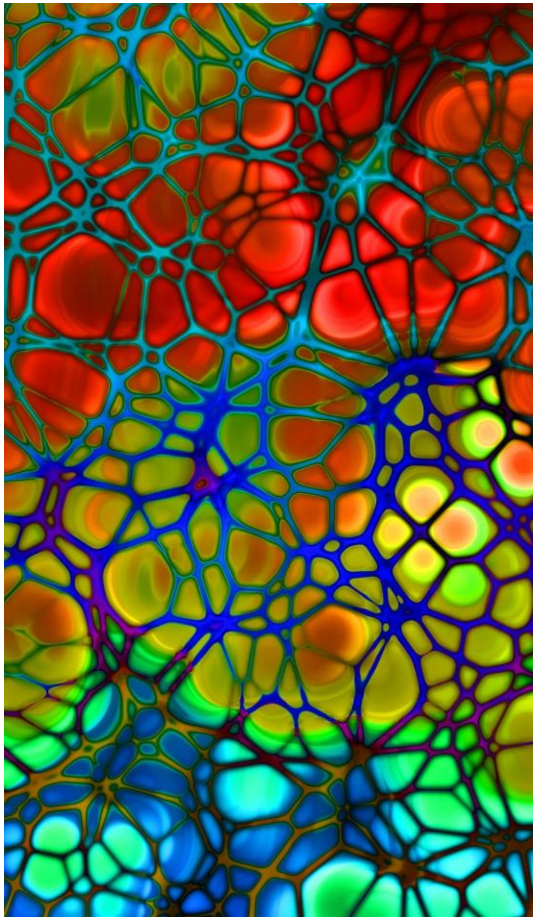
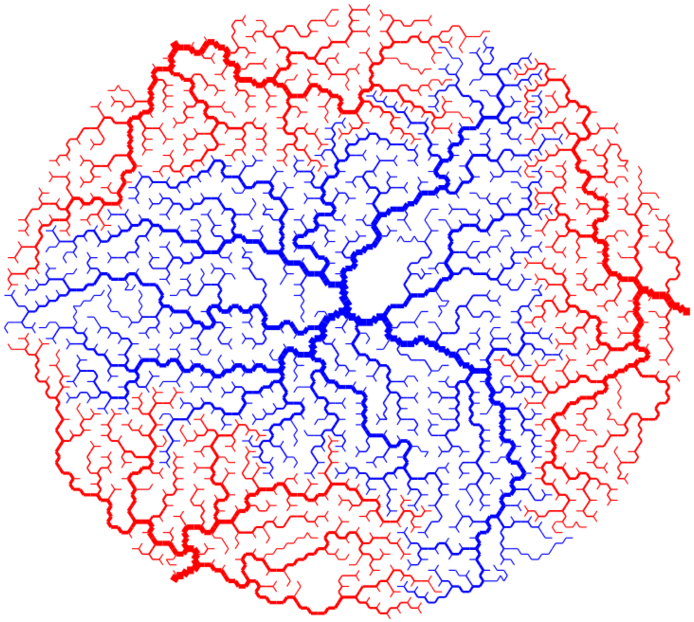
Importance of *in silico* studies on vasculature dynamics

- structure of circulatory network
  - strongly influence living organisms development and functioning
  - hallmark of numerous diseases and pathological states
- problems with *in vivo* & *in vitro* methods
  - cost of obtaining data (time, resources, effort)
  - low results reproducibility and accessibility
- impact on other fields of science
  - complex network analysis

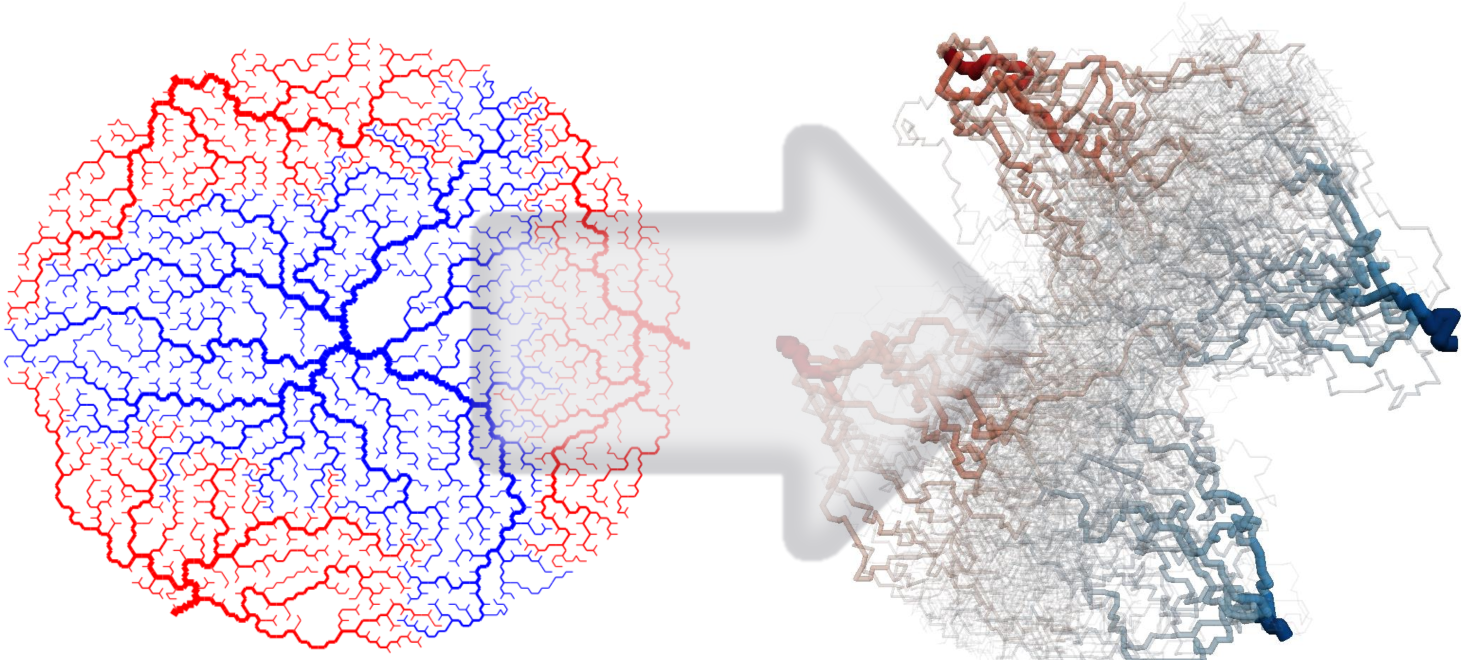


Graph-based vascular model

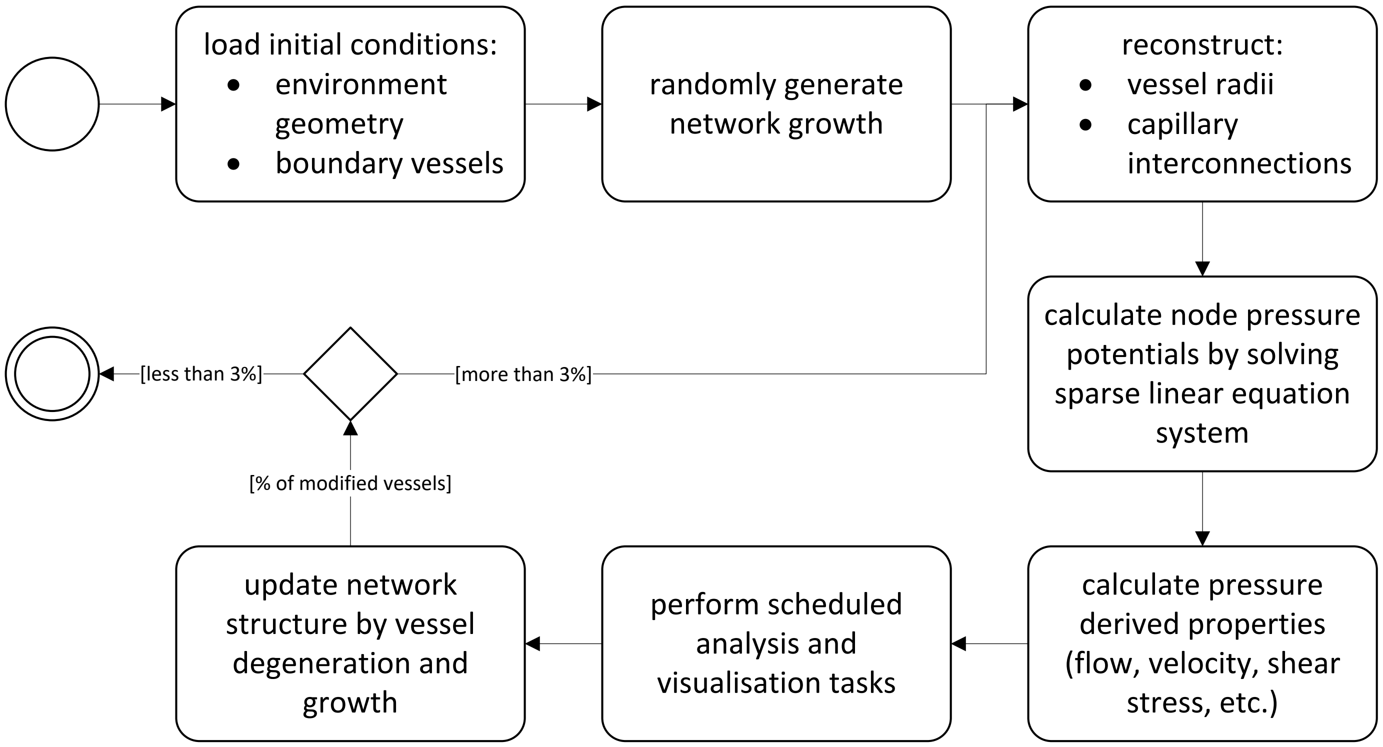


- Ralf Gödde & Haymo Kurz: „Structural and biophysical simulation of angiogenesis and vascular remodelling” *Developmental Dynamics, 220(4):387–401, 2001*
- proposed model:
  - network limited by a predefined fixed grid
  - segment-driven random growth
  - refinement based on underlying physics
- restricted to two dimensional scenarios only

Towards 3-D generalisation

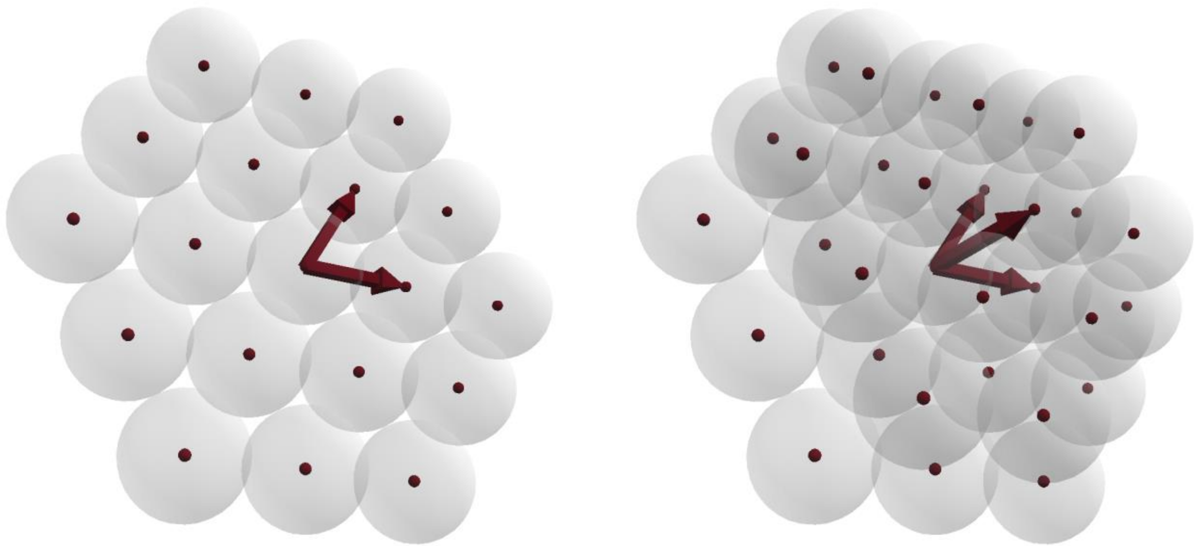


Proposed workflow



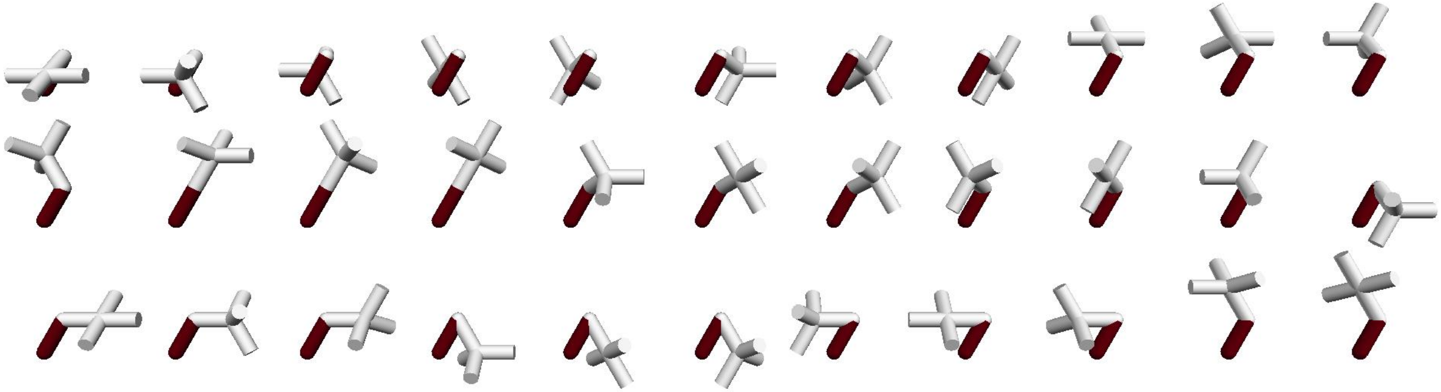
Generalising the concept of fixed simulation grid

- pattern emerging from close packing of spheres
  - inspired by soap-film junctions and honeycomb arrangement of living cells
- hcp lattice 3-D grid used as an equivalent of the hexagonal 2-D grid



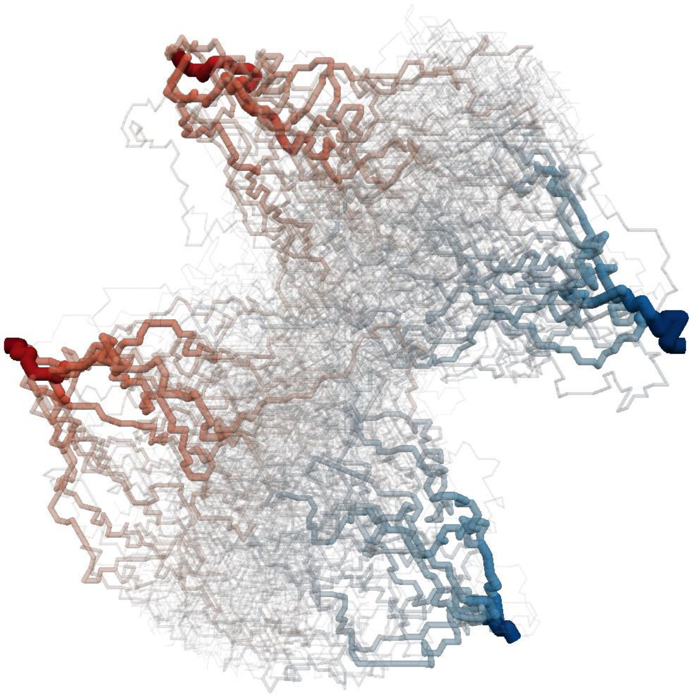
Generalising the concept of building segments

- 33 possible elementary building blocks instead of just 1
- derived from a neighbourhood exploration principle
- should all of them be allowed?
  - versatility and possible networks space
  - minimal bifurcation angle (120° or 107° or 90° ?)

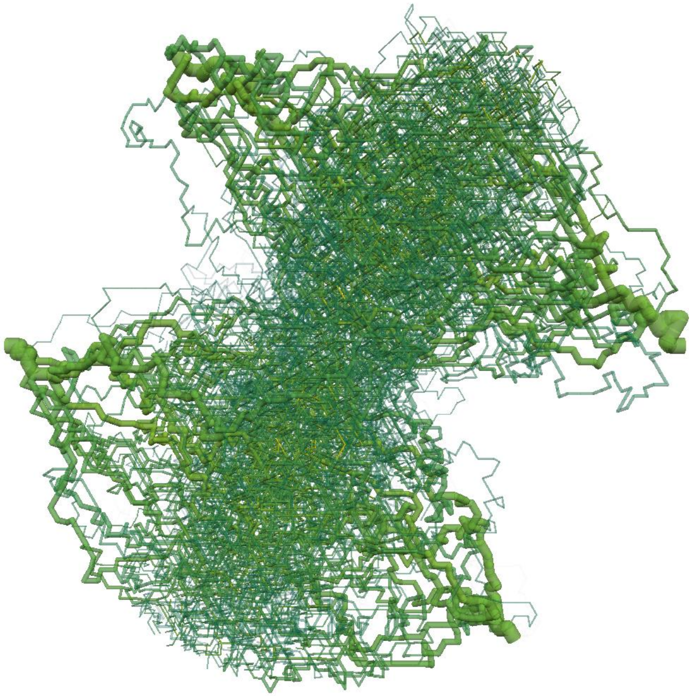


Preliminary results

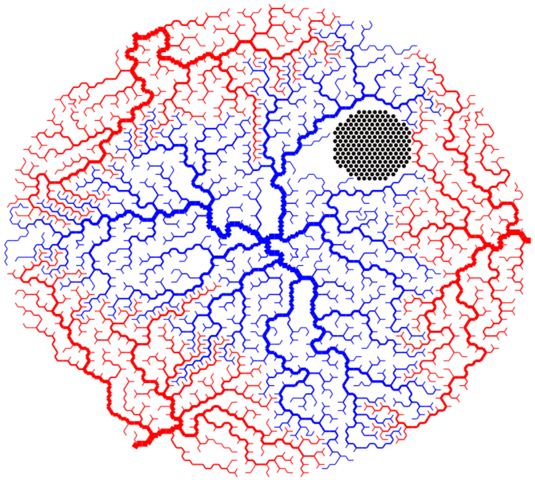
sample result

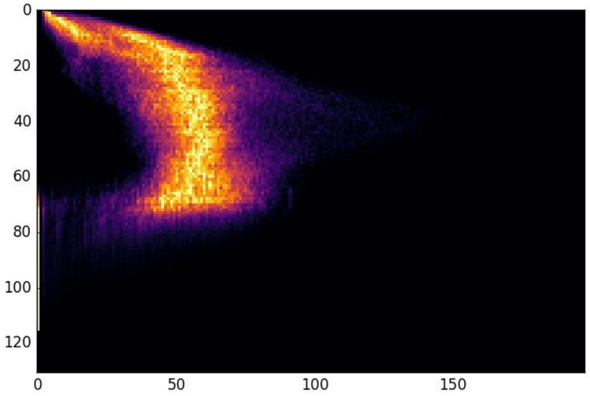


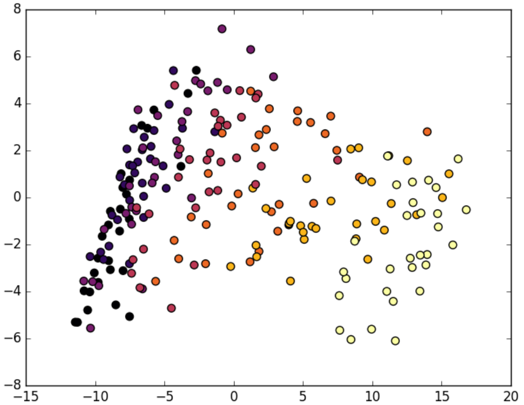
shear stress distribution

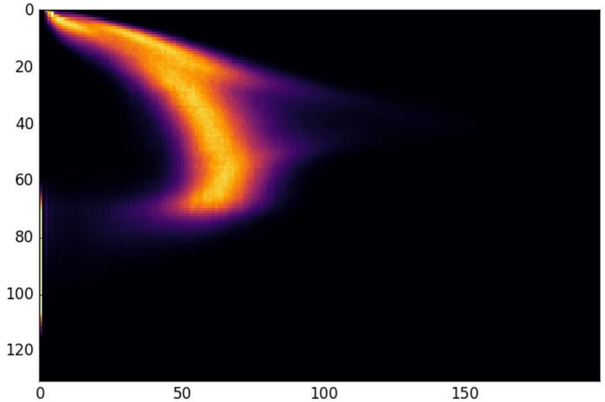


B-Matrix investigations of the obtained networks

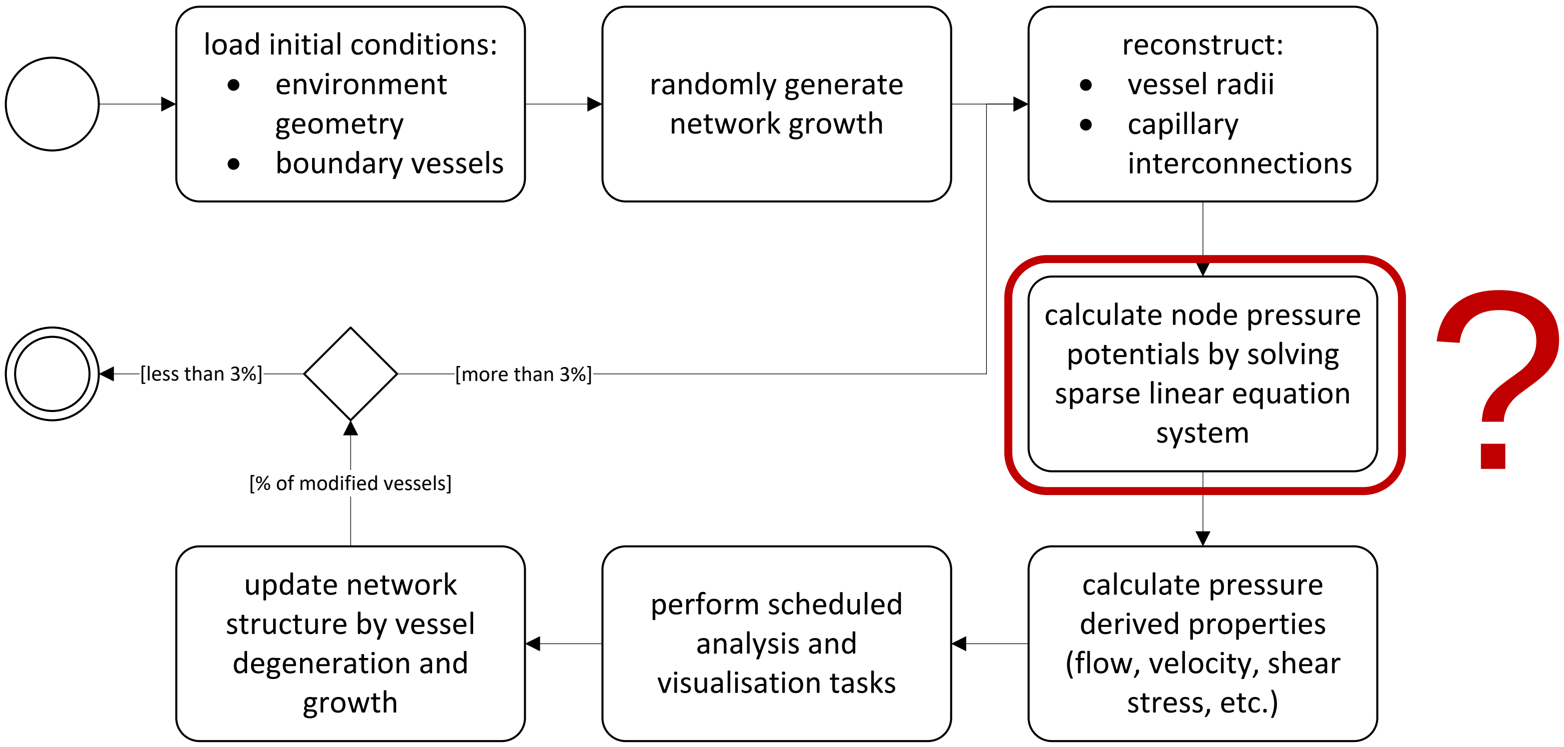








Discovered challenges and bottleneck points



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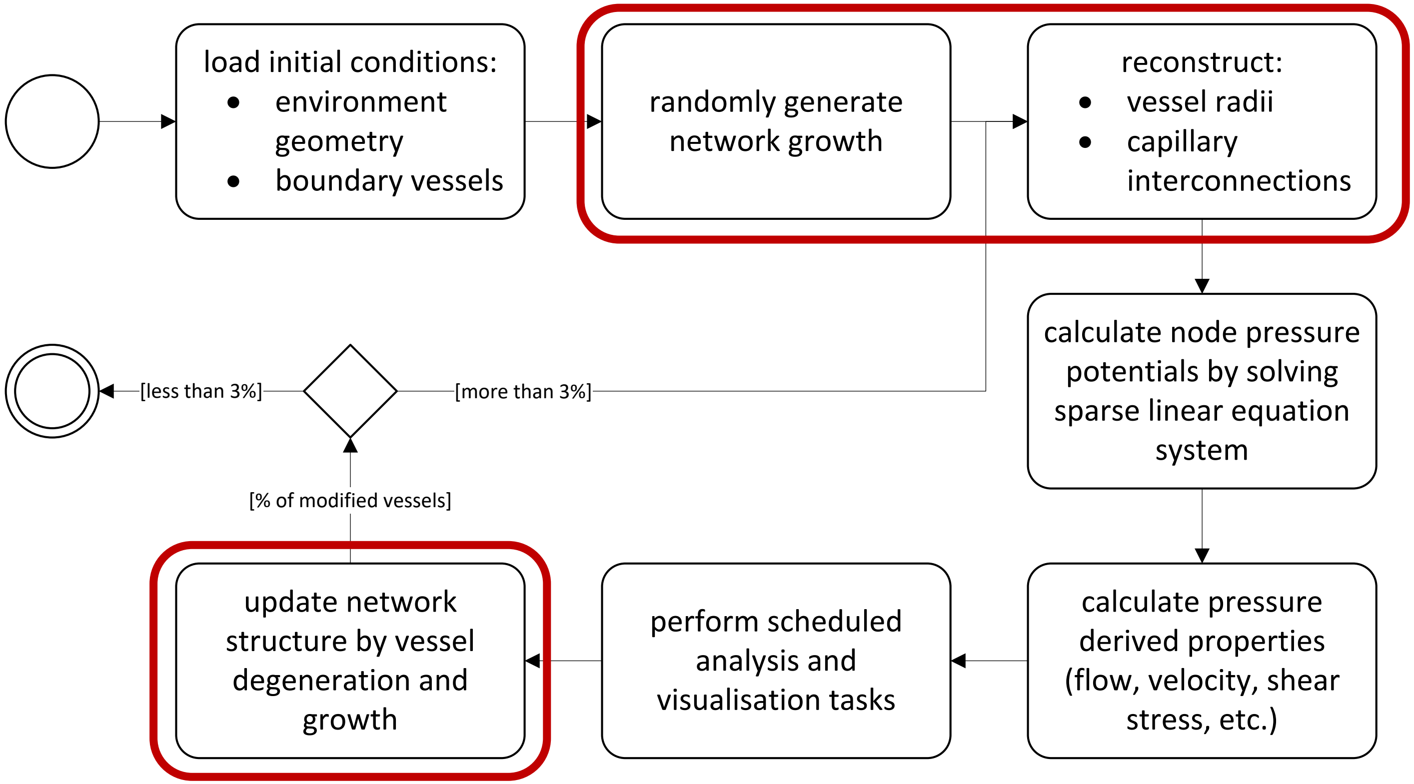

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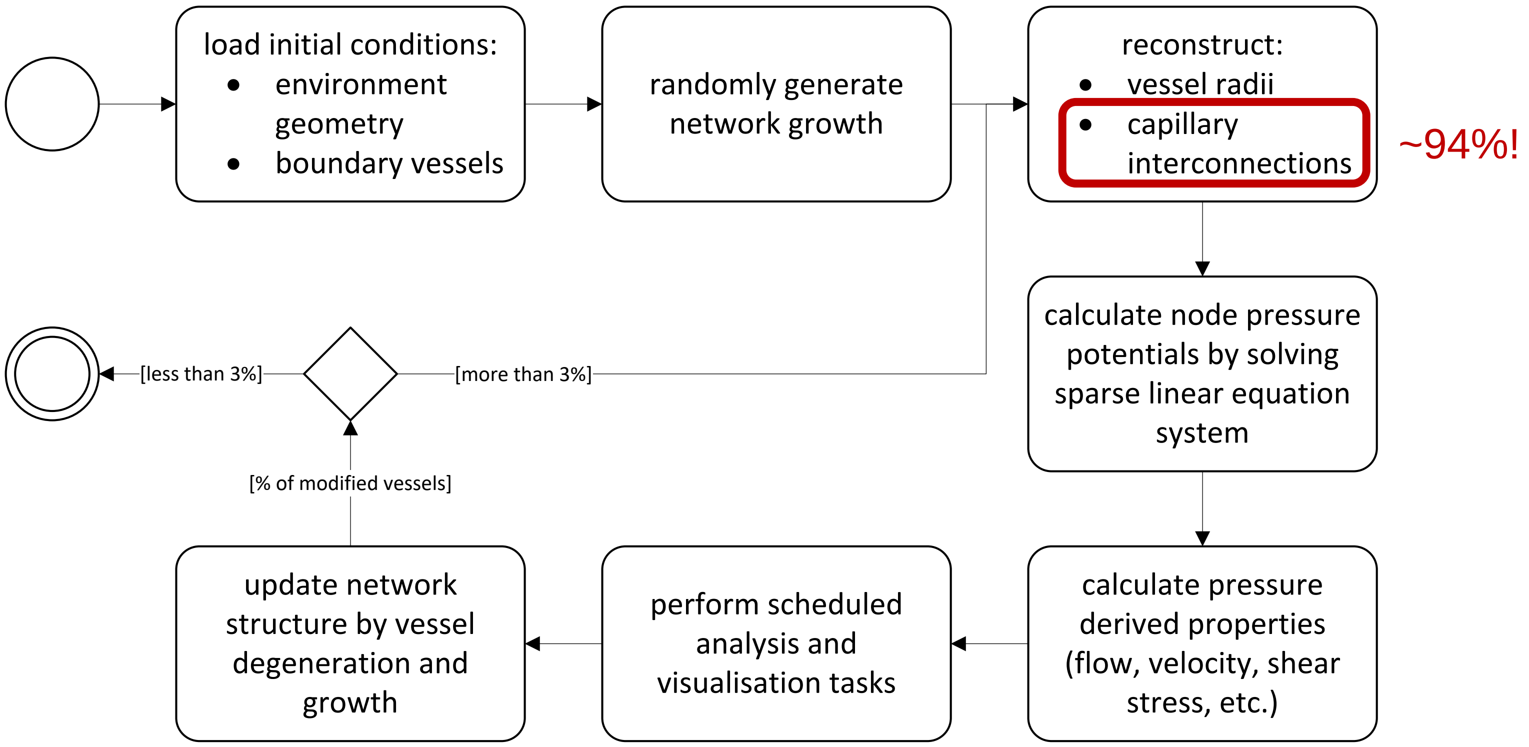

Discovered challenges and bottleneck points

- time complexity tend to scale linearly with the number of nodes N
- N depends on the simulation area radius and number of dimensions

$$N \sim r^d$$

- growth of the neighbourhood size scaling coefficient
  - from 6 to 12 in single step case
  - from 18 to 54 in double step case
- map-reduce parallelisation?
  - optimal grid partition problem
  - not every step is independent (collision avoiding policy)
  - caching

Conclusions

- the proposed model yield plausible results and is a promising basis for future research
- adopting the graph-based paradigm resulted in a range of benefits…
  - robust framework for future enhancements
  - no risk of artefacts occurring due to floating-point geometry
  - output suitable for complex network analysis
- …although not without a cost
  - cohesion management delegated to the graph operations level
  - problems with efficient parallelisation

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