Challenges in 3-D simulation of vascular graph remodelling

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Acknowledgements This research is financed by the Polish National Center of Science (NCN), project DEC 2013/10/M/ST6/00531
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


- 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

load initial conditions:
- environment geometry
- boundary vessels

randomly generate network growth

reconstruct:
- vessel radii
- capillary interconnections

calculate node pressure potentials by solving sparse linear equation system

calculate pressure derived properties (flow, velocity, shear stress, etc.)

update network structure by vessel degeneration and growth

perform scheduled analysis and visualisation tasks

update network structure by vessel degeneration and growth

[less than 3%] - [more than 3%]

[percent of modified vessels]
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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- Reconstruct:
  - Vessel radii
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- Calculate node pressure potentials by solving sparse linear equation system

- Calculate pressure derived properties (flow, velocity, shear stress, etc.)

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Discovered challenges and bottleneck points

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- randomly generate network growth
- reconstruct:
  - vessel radii
  - capillary interconnections
- calculate node pressure potentials by solving sparse linear equation system
- calculate pressure derived properties (flow, velocity, shear stress, etc.)
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- update network structure by vessel degeneration and growth
- [less than 3%]
- [more than 3%]
- [% of modified vessels]
- [94%]
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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