A Distributed GPGPU-based Multiscale Modelling Framework for Complex Systems

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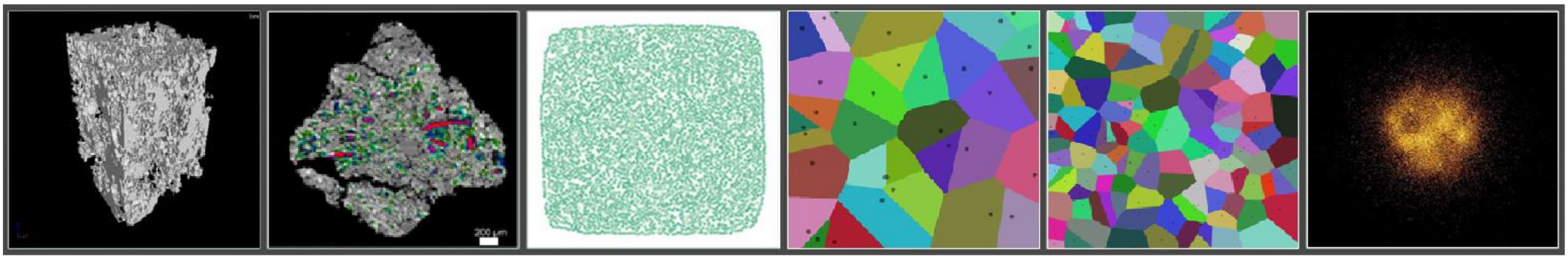


Project Aims

Soil Biophysics

Link microbial processes occurring at relevant scales (µm) to properties measured at soil core (cm) scale (CO_2 respiration)

- 64 million voxels @ 30 micron resolution = 1.2cm^3 soil in which microbes (0.2 – 16 µm)
- 4 months microbial degradation
- 16 hours of simulation

Cancer Systems Biology

Operate at cellular level to observe response at tissue scale.

- 1 million individual cells
- 6 months biology
- 1 week of simulation

Expose similarities of complex systems to develop a modelling framework capable of working across the spatial scales.

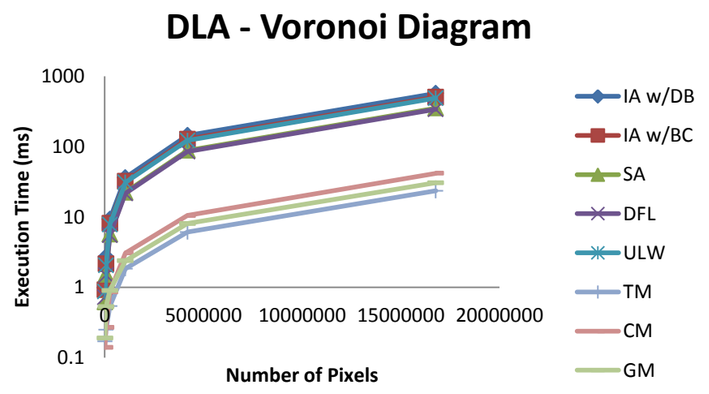
Capable of processing many millions of elements.

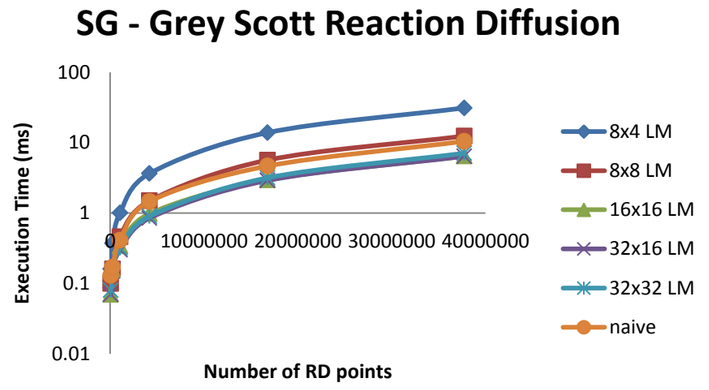
Methodology

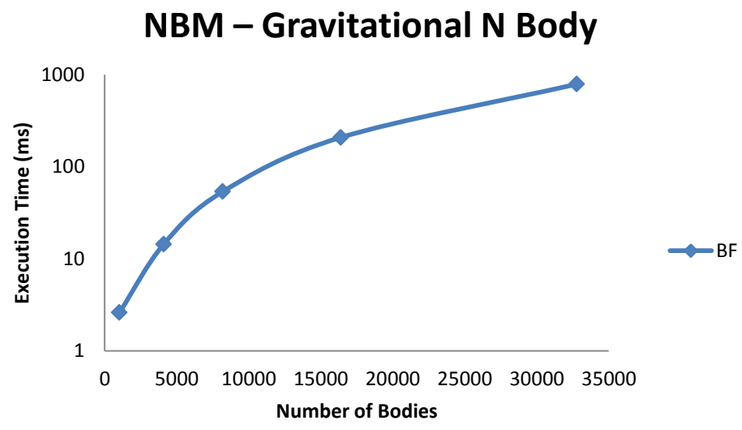
Investigate the “Dwarfs” of most relevance to problem space for different implementations and potential optimisations.

- Dense Linear Algebra
  - involves vector and matrix operations of various complexity
- Structured Grid
  - computations depend on their neighbouring elements
- N Body Methods
  - Physical interactions required between particles

Results







Current Work

- N Body with spatial clustering (Based on Barnes-Hut Method)
  - Various space partitioning methods
    - Voronoi-based, Quad Tree encoding
  - Space filling curves
    - Morton, Hilbert

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