

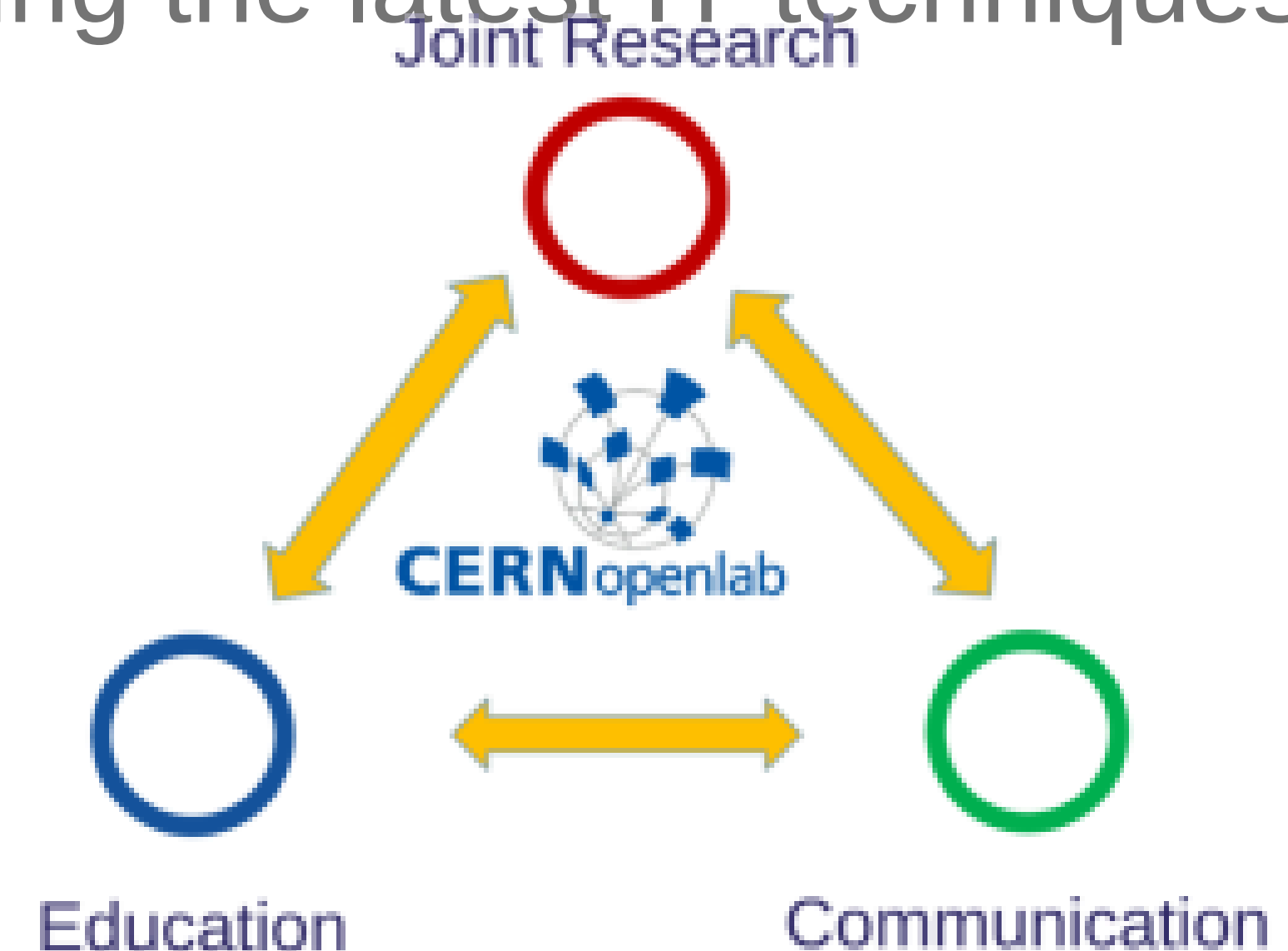


CERN openlab Knowledge Transfer and Innovation Projects

Fons Rademakers, CERN openlab Chief Research Officer
CHEP'16, San Fransisco, 10-Oct-2016.

CERN openlab

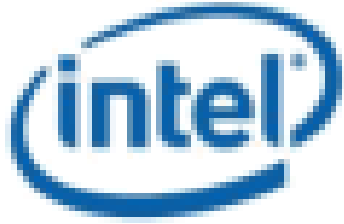
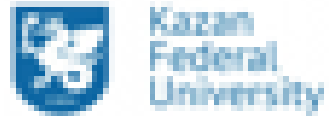
- CERN openlab, a science – industry partnership to drive R&D in IT
- CERN openlab is a driver of innovation, education and entrepreneurship in IT
- Working on multi-disciplinary projects exploiting the latest IT techniques
- Development of educational projects
- Dissemination of results



15 Years of Successful Collaborations



Current CERN openlab Members

Partners	  				
Contributors					
Associates	  				
Research	    				

CERN openlab Knowledge Transfer and Research Projects

- New line of CERN openlab activities
- Investigate how HEP knowledge, methodology and technology can benefit projects in other sciences
- Involve our industry members where possible



The Human Brain Development Project



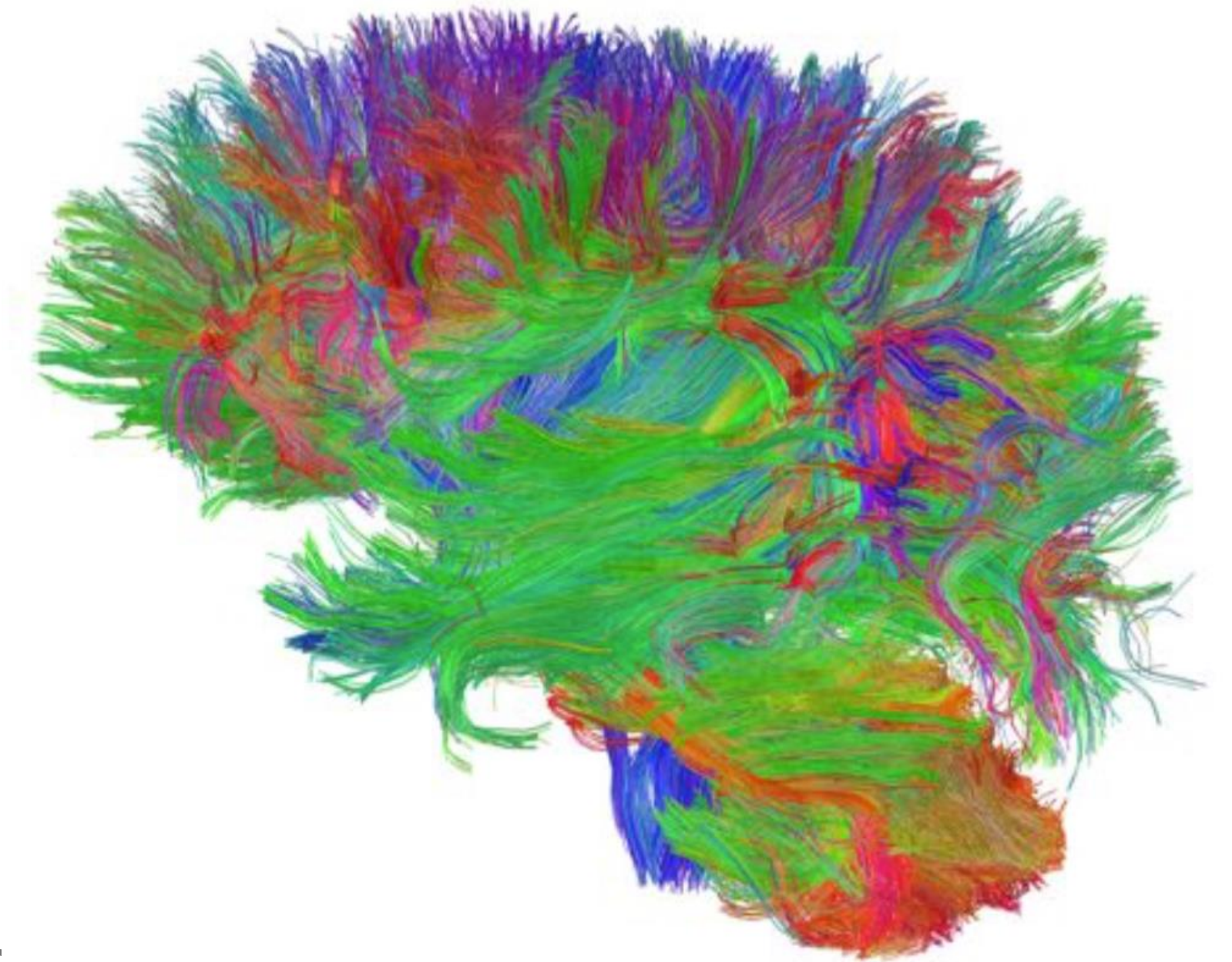
Why Simulate Brain Development

- Neuro scientific insights
 - How does the brain develop?
 - How do genetic and environmental cues interact?
 - How do neurons and brain regions communicate?
 - How does cognition, planning and memory work?
- Medicine
 - Understanding of brain diseases (epilepsy)
 - Tumor growth
 - Drug development
- Technology
 - Artificial intelligence, neural computations, intelligent systems



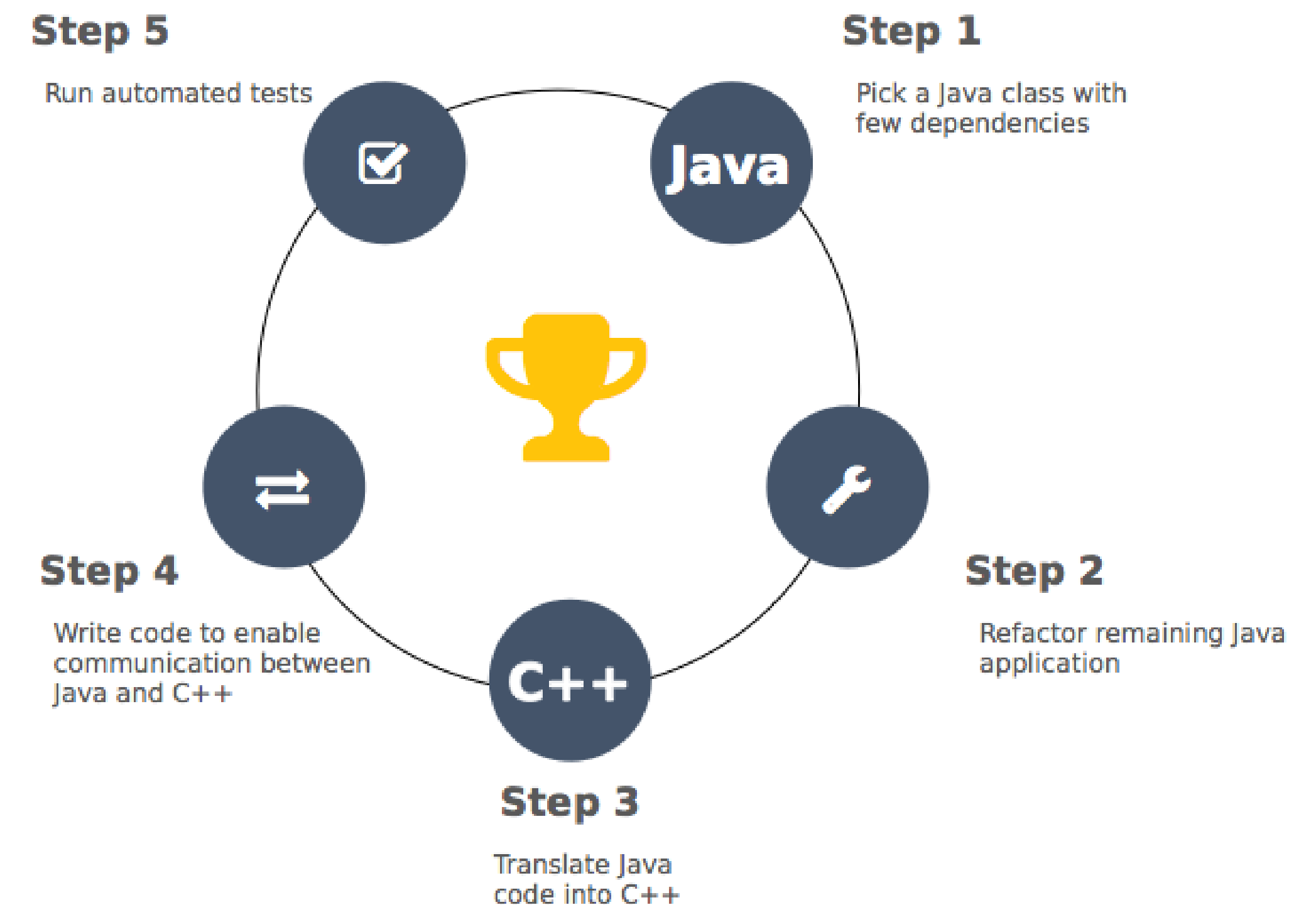
BioDynaMo — The Biology Dynamic Modeller

- Platform for high-performance computer simulations of biological dynamics
- Involves detailed physical interactions in biological tissue
- Highly optimised and parallelised code
- To be run both on HPC and Cloud environments
 - Cortical column: 10k neurons - brain cancer (multi-core)
 - Cortical sheet: 10m neurons - epilepsy (HPC)
 - Cortex: 100m - 10bn neurons - schizophrenia (HPC on Cloud?,

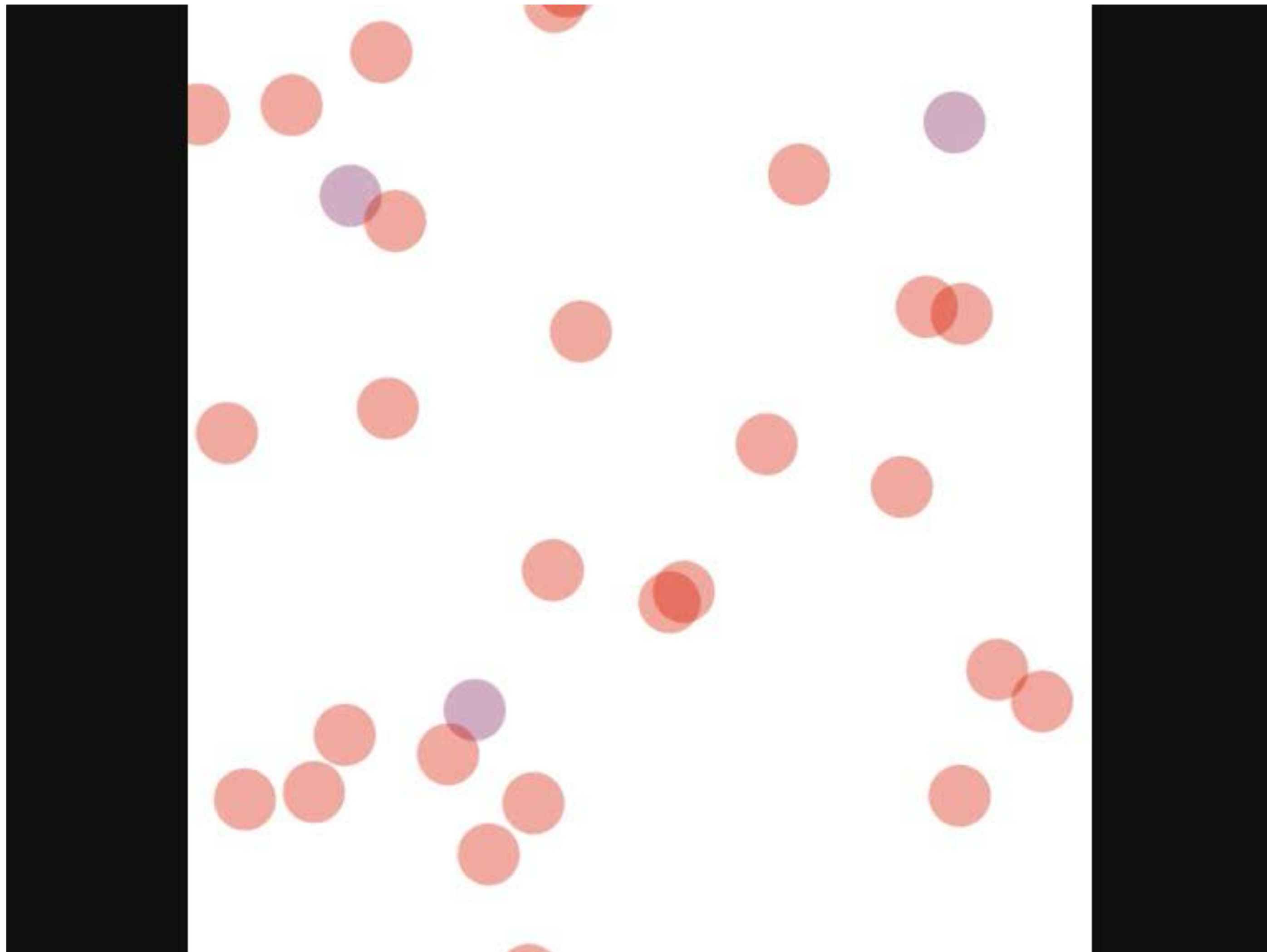


From Cx3D to BioDynaMo

- Original Cx3D code in Java (20 kLOC)
- Ported to C++
- Scalar, serial optimisations
- Vectorisation
- Parallelisation
- Co-processor and GPU optimisations
- ROOT for I/O and graphics



Neurite Growth Simulation with Cx3D



State of the Art Software Engineering Environment

- C++14
- Google C++ coding standards
- Doxygen for source code documentation
- cmake for configuration and building
- GitHub for source code management and issue tracking
- GitBook for documentation
- Travis CI for continuous building and testing
- Slack for instant communication and CERN e-groups for mailing lists

Vectorisation & Parallelisation

- Evaluation of options
 - Auto vectorisation, intrinsics library
 - Compared Vc and Eigen
- Implementation uses abstraction to plugin different Vector Backends (Vc, UMESimd, ...)
- Memory Layout Transformations AOSOA
- Scalar version implemented with ScalarBackend
- OpenMP on operation level

```
template <typename Backend>
class Cell {
public:
    using real_v = typename Backend::real_v;
    using real_t = typename Backend::real_t;
    using bool_v = typename Backend::bool_v;
```

```
struct ScalarBackend {
    typedef Vc::SimdArray<int, 1> int_v;
    typedef Vc::SimdArray<double, 1> real_v;
    typedef double real_t;
    typedef std::array<bool, 1> bool_v;
    static const size_t kVecLen = 1;
};
```

```
void Compute(daosoa* cells) const {
    #pragma omp parallel for
    for (size_t i = 0; i < cells->vectors(); i++) {
```

Refactoring

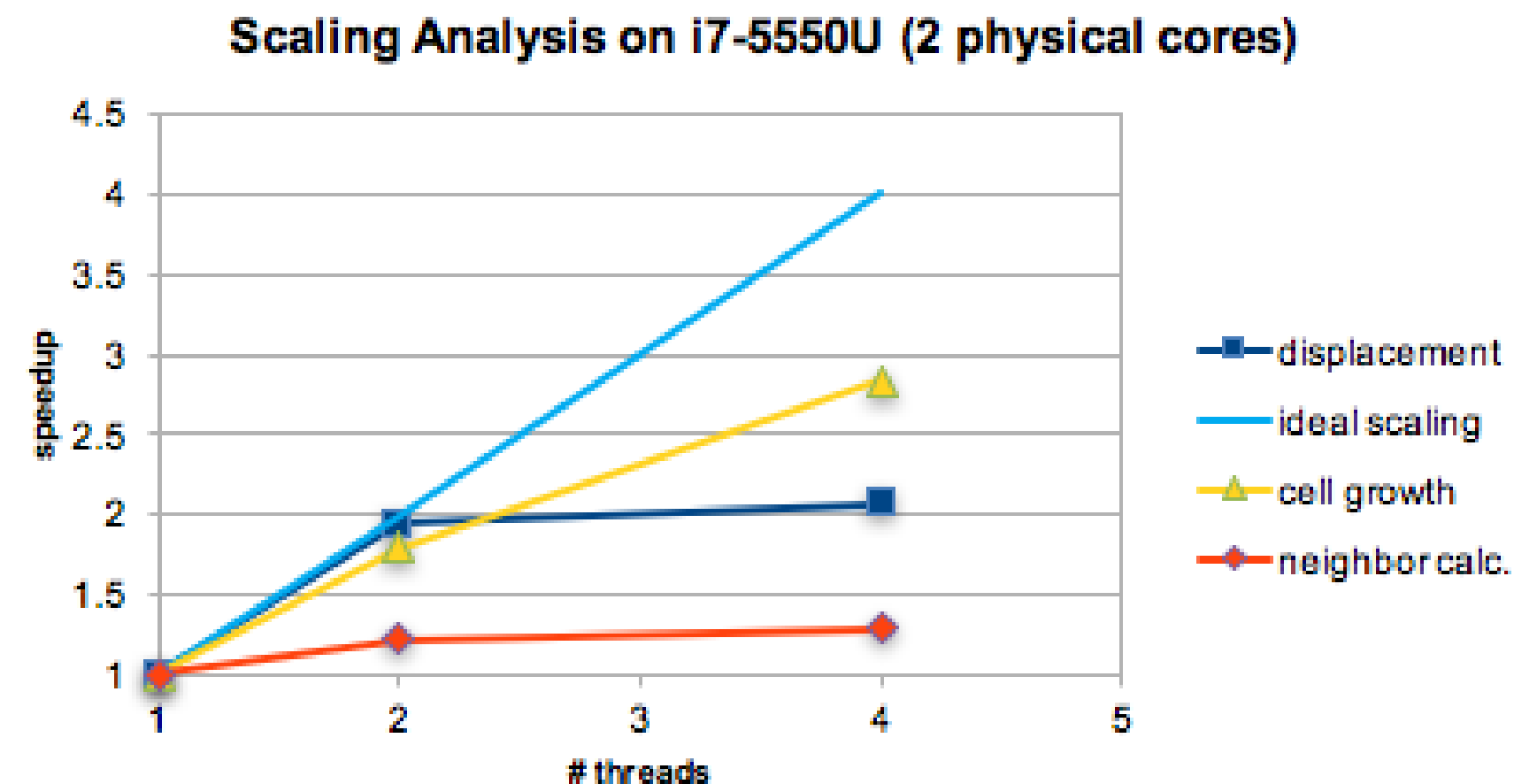
- Extension and modification of classes solved with mixins and variadic templates
- Removed separation of Cell, CellElement, Physical
- Introduced abstraction of an operation e.g. calculation of mechanical forces, neighbours, biological behaviours, ...
- Scientist defines operation graph, runtime figures out dependencies and schedules accordingly (to be implemented)

```
// customize Neuron (add attribute foo_ and member function GetFoo)
template <typename Base>
class NeuronExtension : public Base {
    double foo_ = 3.14;
public:
    template <class... A>
    explicit NeuronExtension(double foo, const A&... a)
        : foo_{foo}, Base(a...) {}
    NeuronExtension() = default;
    double GetFoo() const { return foo_; }
};

// define CustomNeuron
typedef NeuronExtension<Neuron<BaseCell>> CustomNeuron;
```

Preliminary Results

- Example of cell growth, calculation of mechanical forces and neighbours



- Comparison of SSE vs AVX showed a speedup of
 - 1.6x for displacement calculation
 - 1.5x for cell growth

CERN openlab BioDynaMo Technology Transfer Benefits

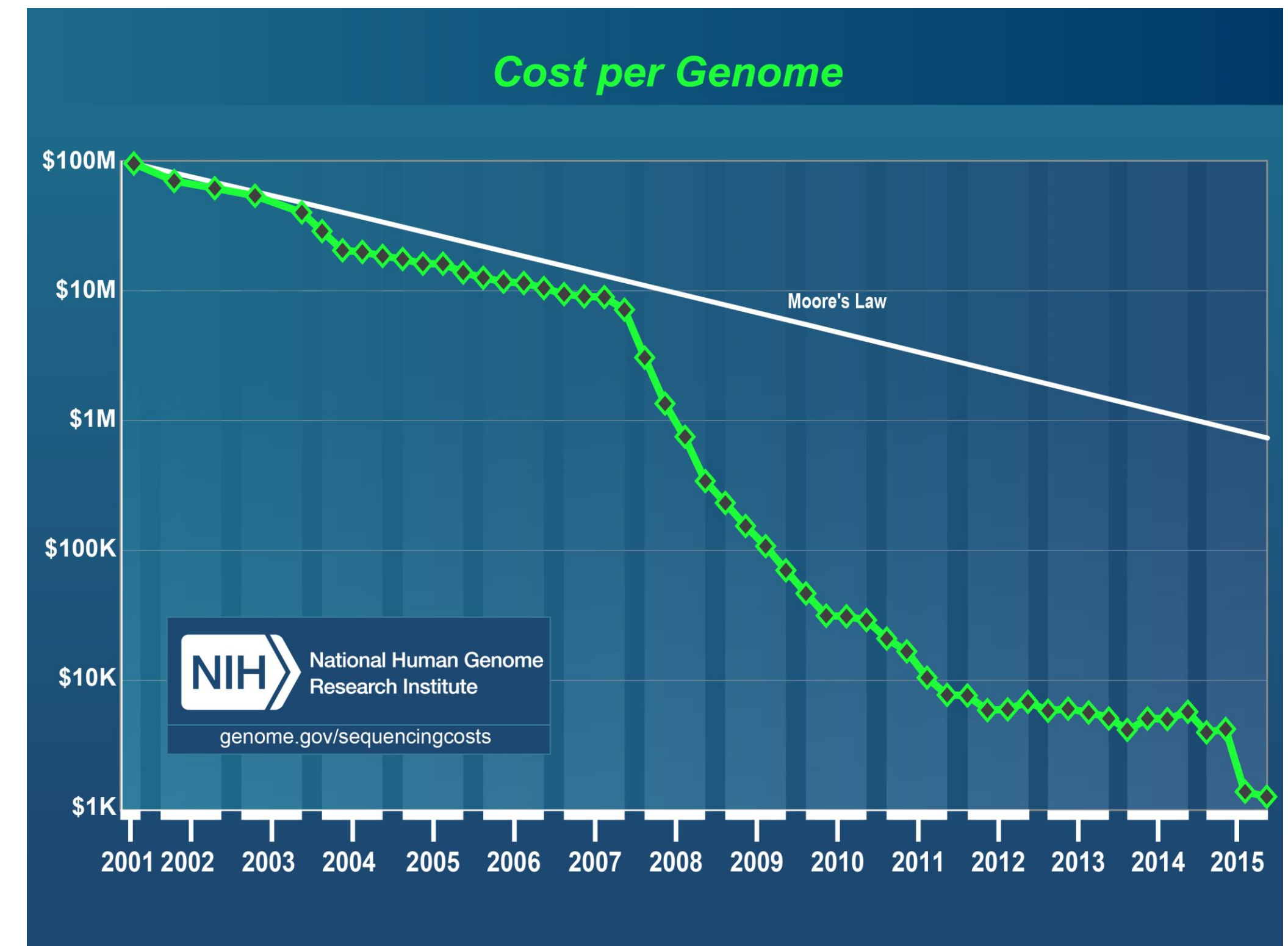
- Ideal project for code modernisation effort, code not too large but very relevant
- CERN openlab provides technical student who gains valuable experience
- Experience very valuable for much larger CERN code modernisation projects
- BioDynaMo code will boost the neuroscience brain simulation capabilities
- Project is joint effort between CERN openlab, CERN medical applications group, Newcastle University, Kazan University, Innopolis University and Intel



Using ROOT for Genomics Data Analysis

Rapidly Increasing Amount of Genomics Data

- Next generation Sequencing (NGS)
- Dramatic increase in the amount of data
- Improved data confidence
- NGS is enabler for more sophisticated research questions in Genomics



Issue: Leaps in sequencing technology have outperformed advances in computing

The TwinsUK Project

- The TwinsUK resource is the biggest UK adult twin registry (more than 11000 twins, 300 TB genomics data)
- Evaluate if the optimised ROOT file format and analysis features are more efficient for this type of studies than BAM and standard genomic analysis tools
- Evaluate Seagate Kinetics key/value storage facility
- Partners
 - Formal interface: King's College London
 - Behind KCL: entire consortium working on Twins UK (~ 50 institutes)

CERN openlab TwinsUK Technology Transfer Benefits

- Additional use case for CERN's ROOT and Seagate's Kinetics technologies
- Return flow of know-how benefiting the ROOT User community
- Entire Omics community would benefit from improved analysis tools to handle rapidly growing amounts of data
- Project is joint effort between CERN openlab, CERN medical applications group, King's College London and Seagate



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