Simulating flexible filaments, motor proteins, and arbitrary rigid bodies using SkellySim

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Introduction to SkellySim

https://github.com/flatironinstitute/SkellySim

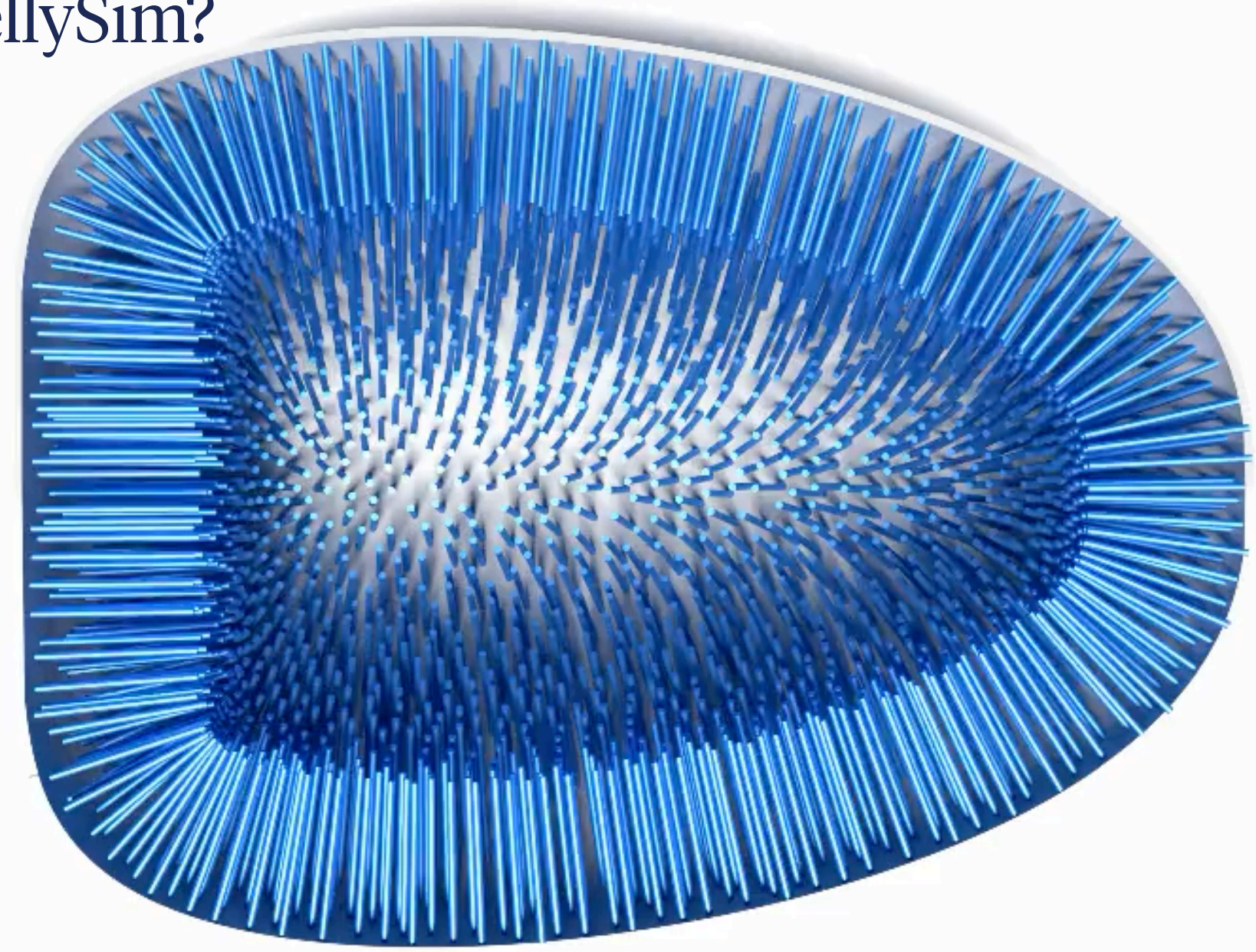
SkellySim

Dutta *et al.*, 2024, *Nature Physics.*

What is SkellySim?

- Cytoskeleton (skelly) simulator (sim)
- Full hydrodynamic simulation of
  - Fibers: Microtubules or other flexible filaments (perhaps with ‘motors' exerting a force-density on filaments and against the fluid)
  - Bodies: Smooth ‘rigid’ objects like organelles or MTOCs
  - Periphery: Smooth/convex containing volume (cell boundary)

Why is SkellySim?



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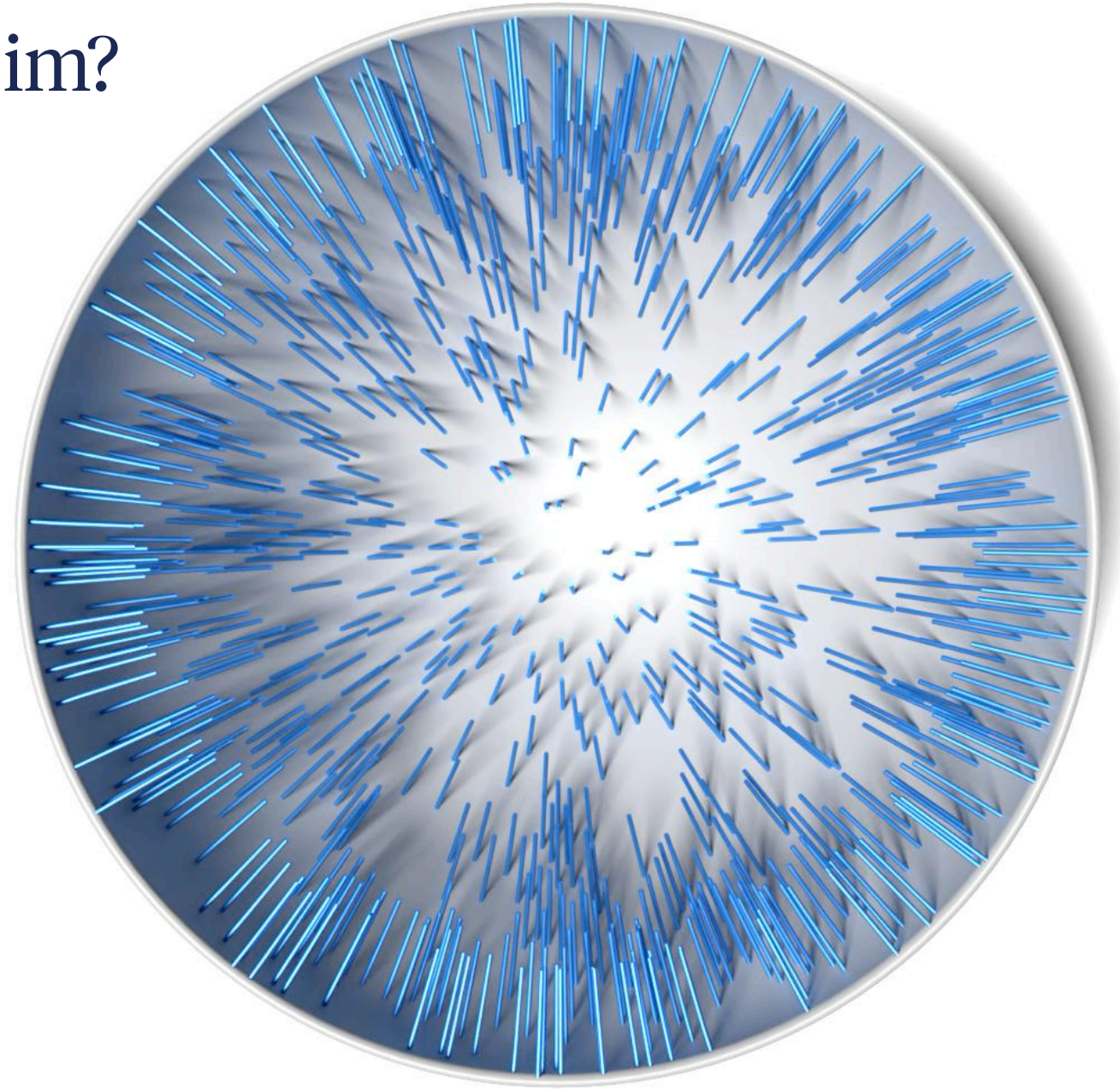


Who is SkellySim?

- High performance code developed by **Robert Blackwell** (Flatiron Institute - SCC) and **David Stein** (Flatiron Institute - CCB)
  - Ground-up re-write of the work in CCB by **Gokberk Kabacaoglu** (now at Bilkent University, Ankara)
  - Which itself was an extension of work by **Florencio Balboa Usabiaga** (now at Basque center for Applied Math)
  - Which itself was based on work by **Ehssan Nazockdast** (now at UNC Chapel Hill)
  - Which itself goes back to work by **Tornberg** and **Shelley**
- Original python code had limited extendability and scalability
- Solver stalled in large and unavoidable external “serial” code portions

SkellySim technology overview

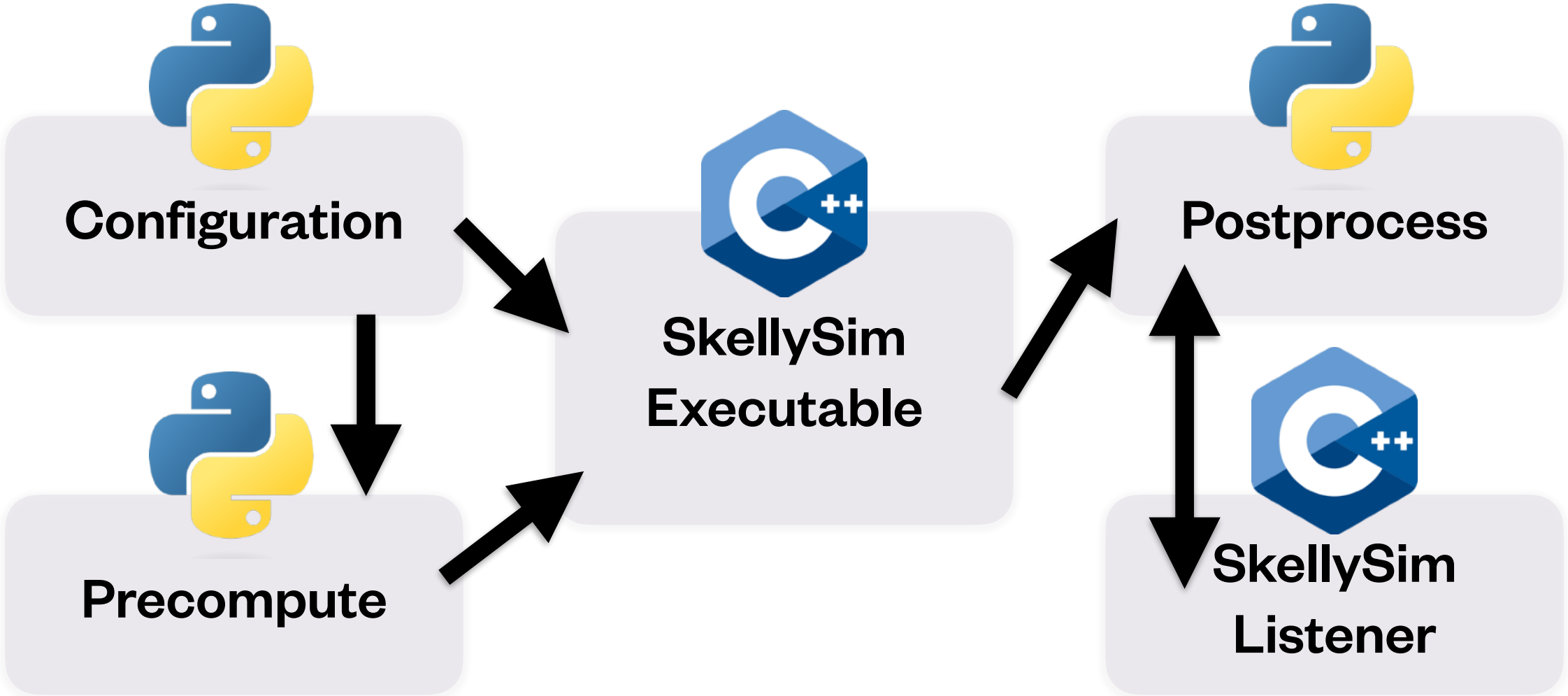
C++

- `MPI` to distribute calculation for simulation objects
- `Trilinos` for `GMRES` solver to resolve “global” matrix equations
- `Eigen` for “local” matrix/vector computations
- `PVFMM/STKFMM` for hydrodynamics calculations
  - `CUDA` and `CPU` direct solvers for smaller systems
- `msgpack` for serialization/inter-language communication

Python

- Frontend for configuration and precompute steps
- Analysis on the backend
- Plugins for `blender` visualization

SkellySim workflow



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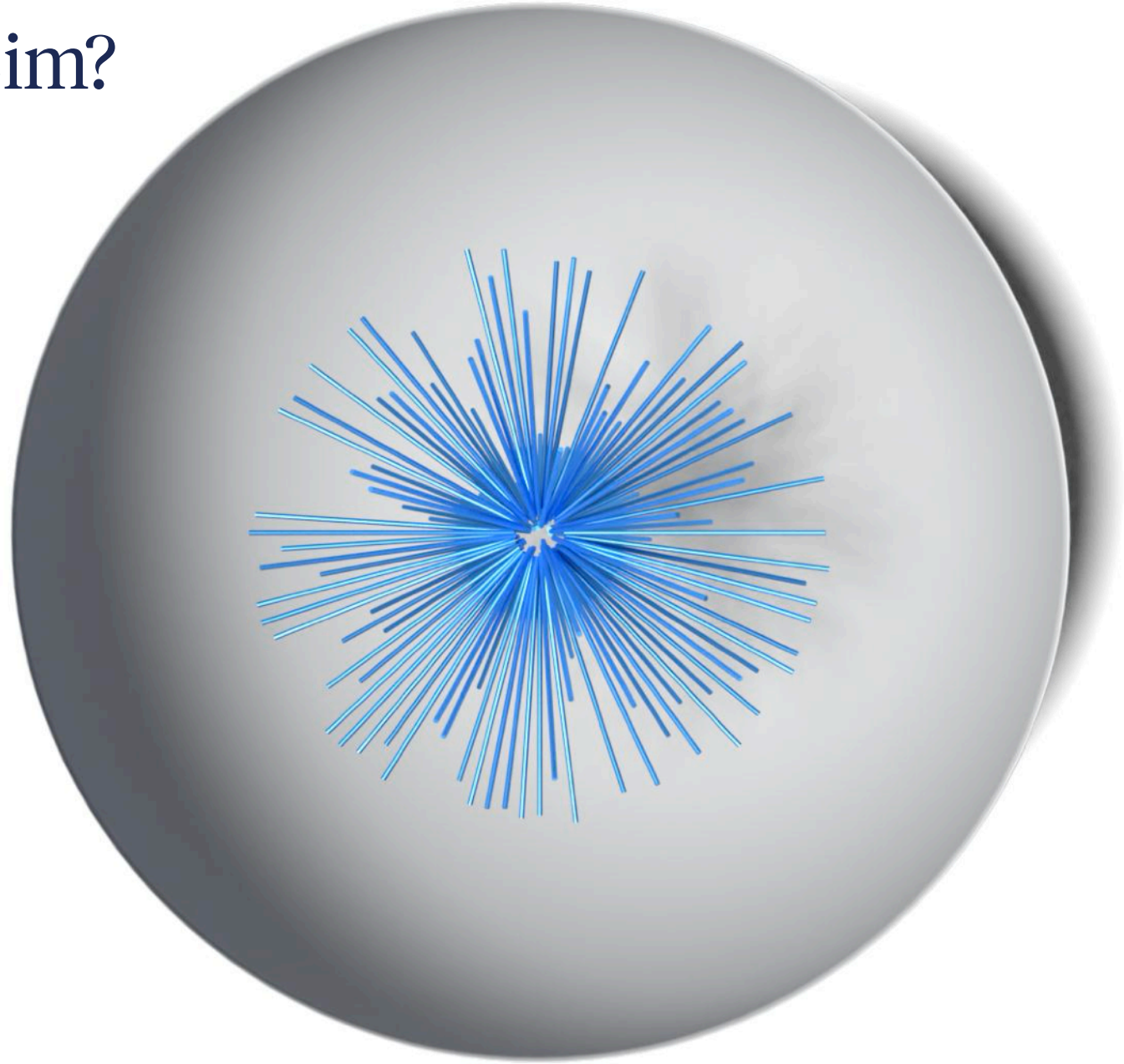

SkellySim Tutorial

SkellySim

https://sdsc-binder.flatironinstitute.org/~cedelmaier/skelly_sim

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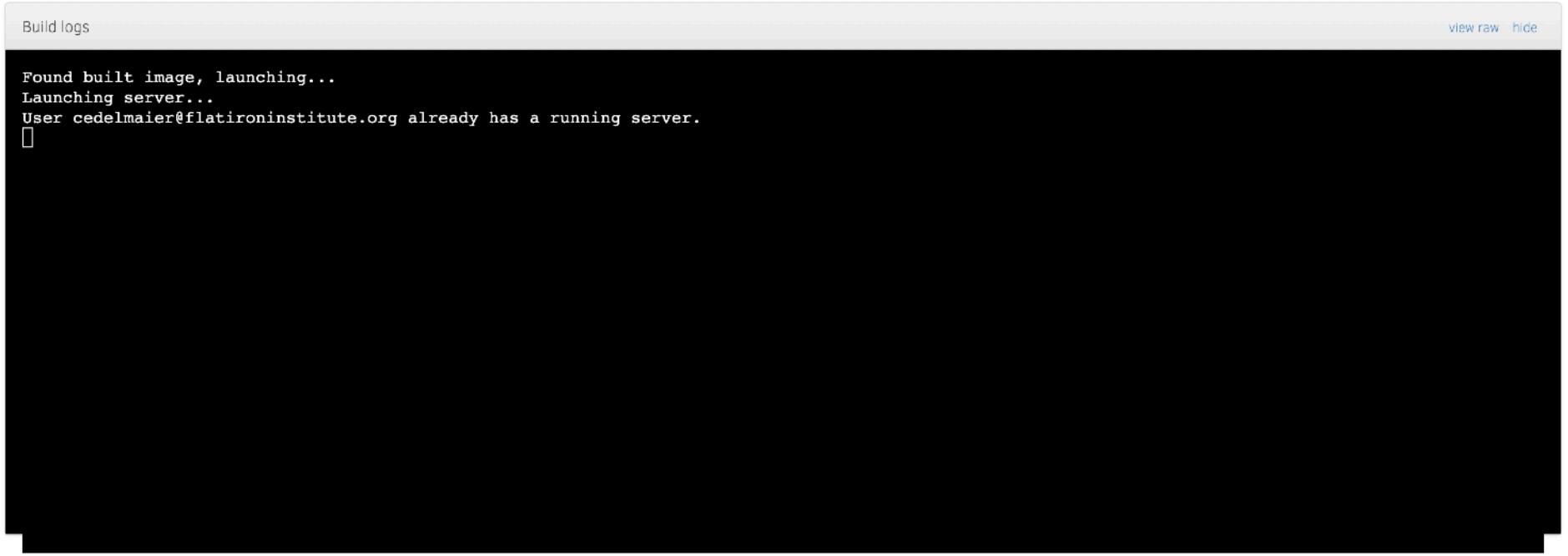
SkellySim



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