Software Architecture Design for Modular Multiphysics Simulations

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Summary

- Achieving the long-term objectives of the TriForce computational environment will require careful attention to software architecture and design from its earliest stages
- The TriForce Fundamental Algorithm Testing Environment (TFFate) is being developed as a stand-alone application in Python to serve as a framework for software architecture prototyping and algorithm development
- Inspired by concepts in general code design and software architecture [1], the principle of an "architectural hierarchy" specific to scientific code development is proposed
- Extensive use of Abstract Base Classes (ABCs) allows for implementation within the architectural hierarchy without sacrificing user extensibility [2]

Objectives of TFFate

For TriForce:

- Provides a staging ground in Python for the addition of new functionalities and algorithms to the primary TriForce computing environment in C++
- Provides a prototype for the long-term architecture of the TriForce computing environment

For the Learner:

- The flow of the code and the role of its parts can be understood using only high-level knowledge of the simulation archetype (PIC, FCV, SPH, etc.)
- Individual parts of the code can be read and understood without detailed knowledge of the rest of the code

1. Simplicity of form without loss of function

For the Developer:

- Individual parts of the code can be added to or modified with as few changes as possible
- Extensive testing suite, along with test-driven development streamlines bug squashing

2. Simplicity of change without loss of stability

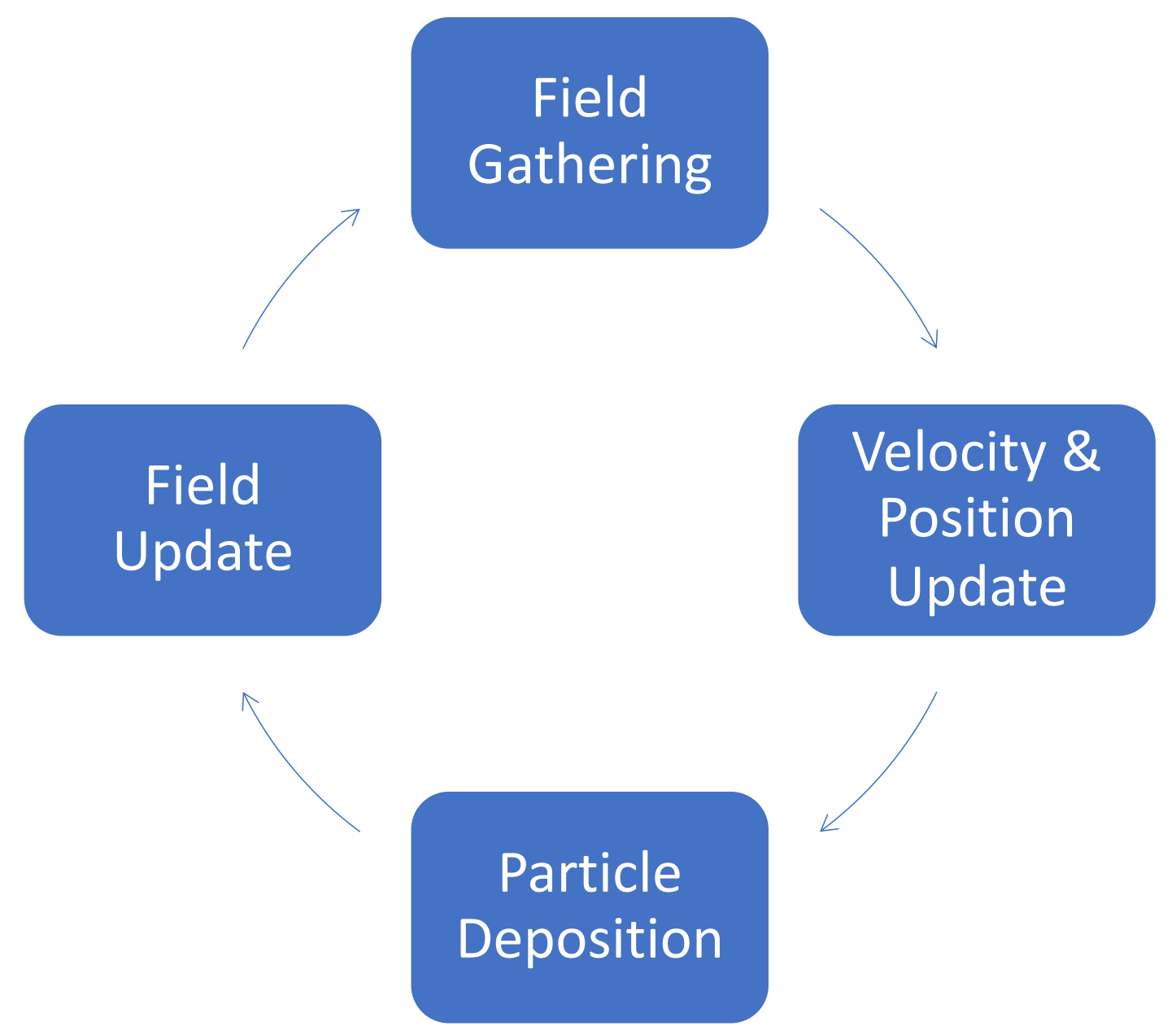
For the User:

- Existing input decks can be read, understood, and modified easily
- For experienced users, simplicity of control does not mean loss of granularity

3. Simplicity of control without loss of granularity

PIC Archetype

Core Particle-in-cell (PIC) Loop



Field Gathering:

- Interpolating field values from the grid to the particles to calculate electromagnetic forces

Velocity & Position Update:

- Integrating the Newton-Lorentz equations of motion to update particle v(t) and x(t)

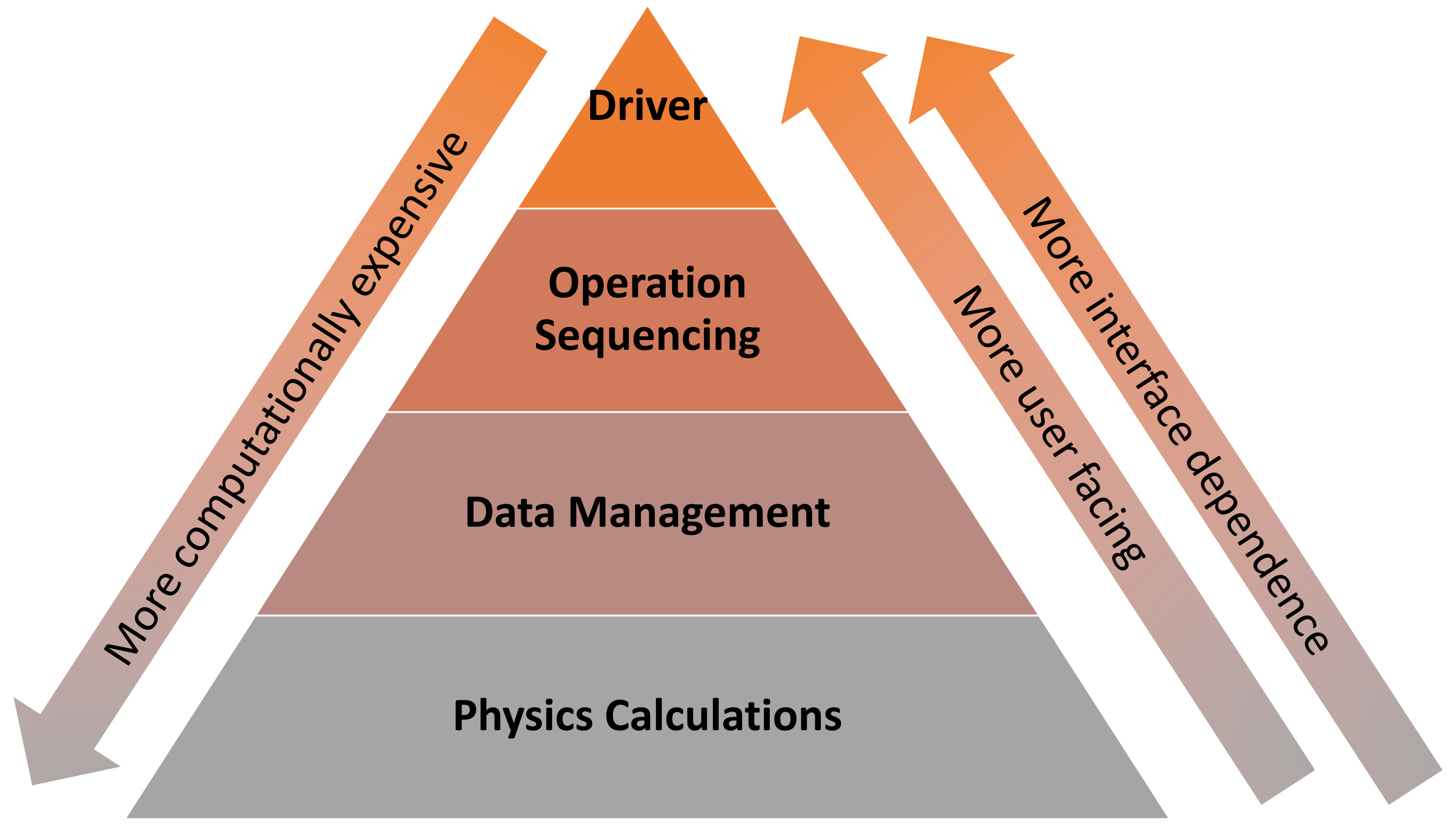
Particle Deposition:

- Interpolating particle charge/current density contributions to the grid

Field Update:

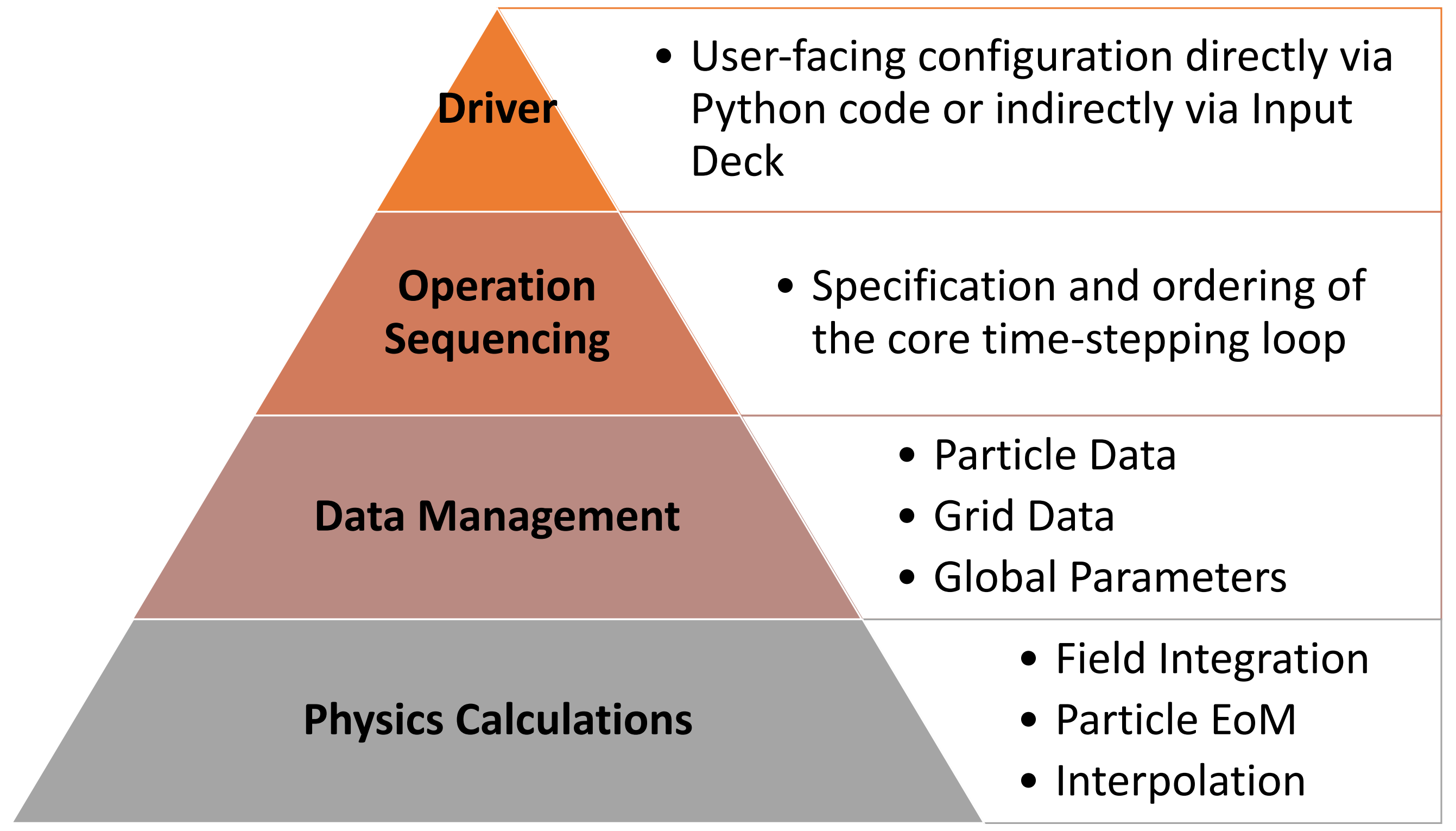
- Integrating Maxwell's equations to update the electric and magnetic fields

Architectural Hierarchy



- Using such a hierarchy as a guiding principle, clarity of structure and modularity of function become natural
- Compartmentalization allows for changes to be localized and encourages modules to be individually intelligible
- Minimizing the impact of intra-code design choices on physics modules allows freedom of implementation and optimization

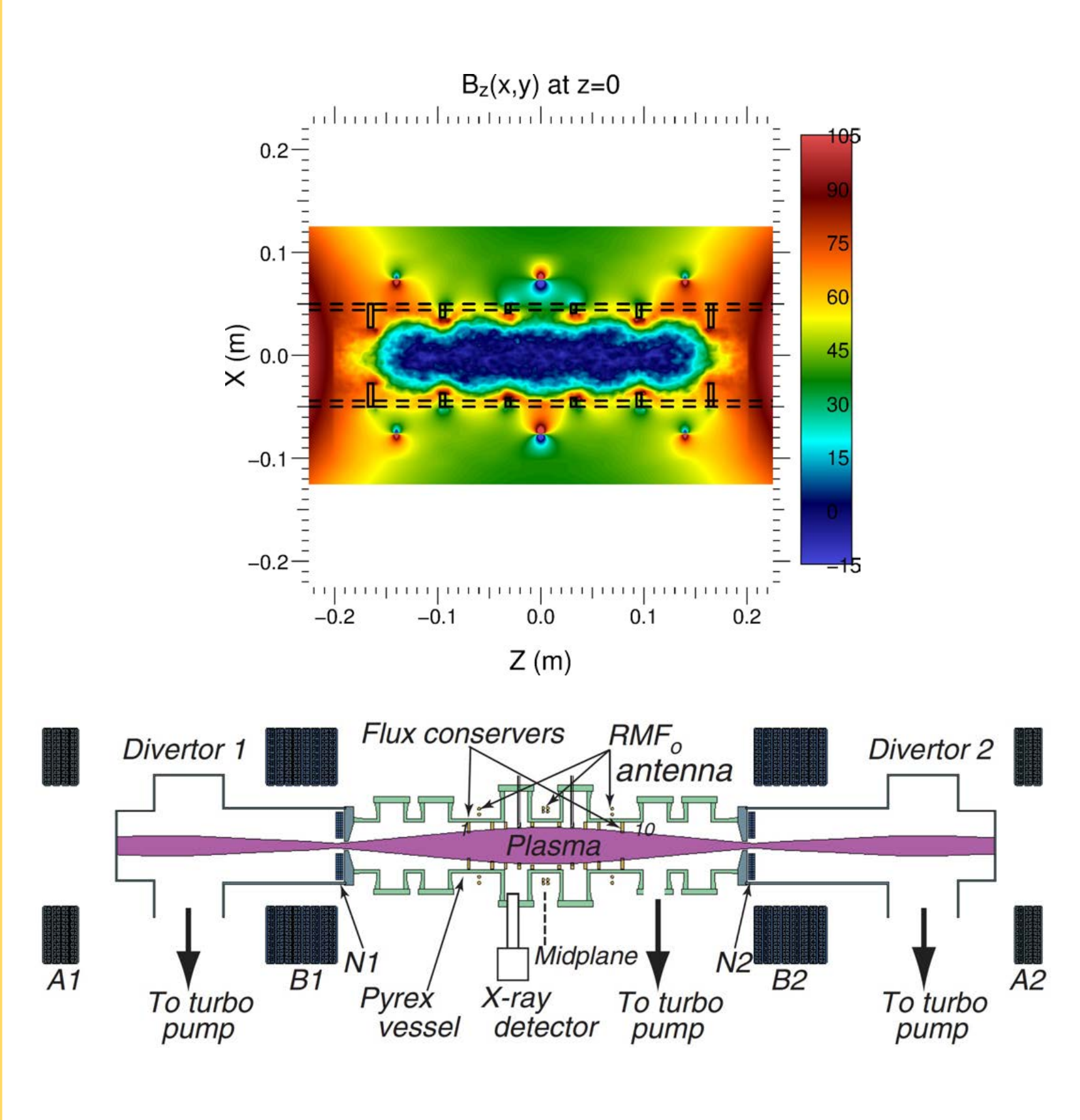
Implementing PIC using the Architectural Hierarchy



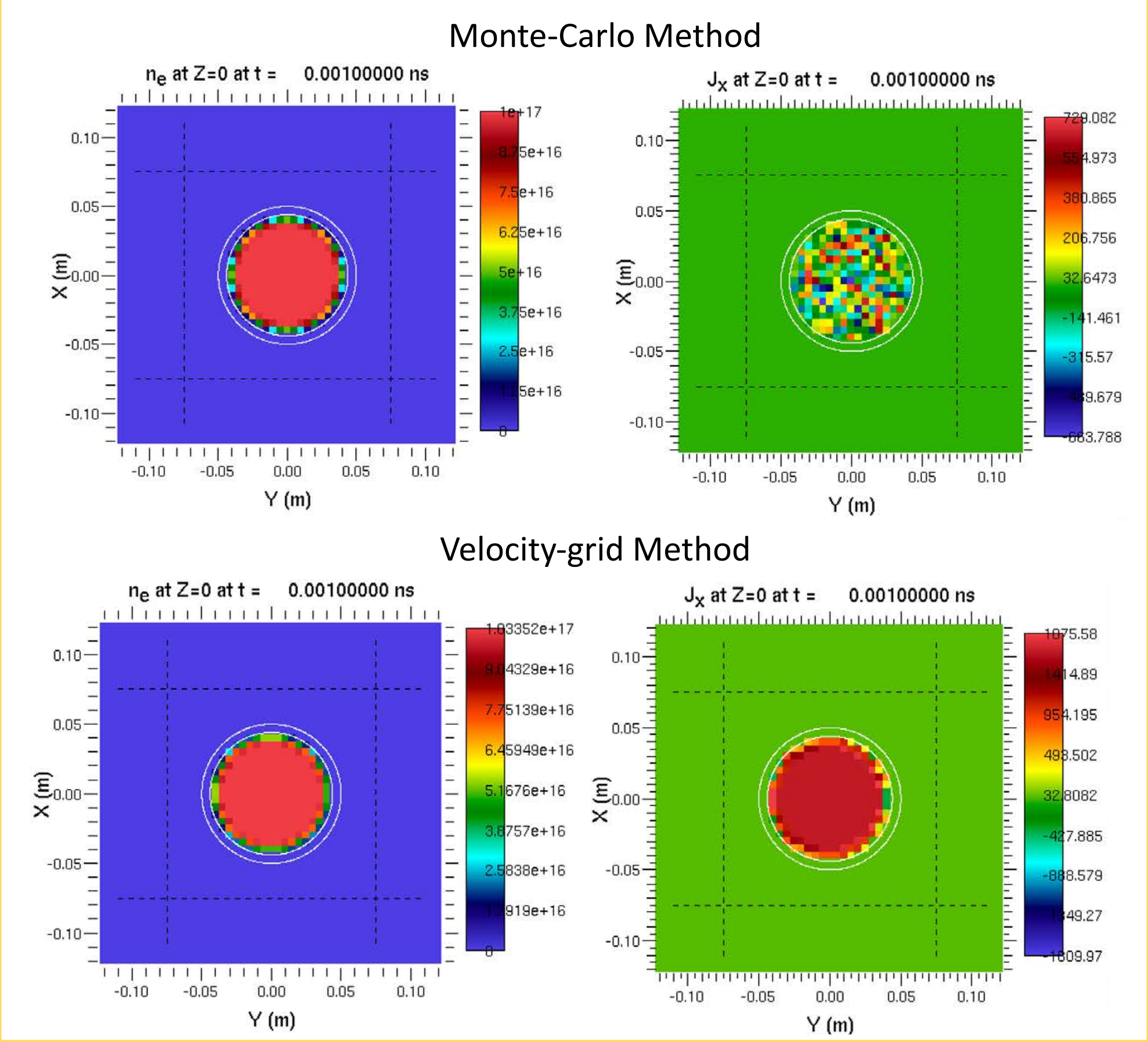
Driver	User-facing configuration directly via Python code or indirectly via Input Deck
Operation Sequencing	Specification and ordering of the core time-stepping loop
Data Management	Particle Data Grid Data Global Parameters
Physics Calculations	Field Integration Particle EoM Interpolation

- Dual configuration schemes allow for simplicity of control without loss of control
- User-defined Sequencers allow simulation archetype to be altered, paving the way for hybrid simulation capabilities
- Compartmentalization of non-physics functionality allows physics algorithms to support modularity

Other Work by TCMM



- TriForce's Library for Integrated Numerical Kinetics (TFLink) is being used in collaboration with PPPL and Princeton Satellite Systems to simulate the PFRC-1 [3] device en route to simulations of PFRC-2/3 (lower figure adapted from [4])


Monte-Carlo Method

Velocity-grid Method

- Novel particle initialization and weighting schemes for reducing particle noise are also being investigated

Next Steps

- Finalize v1.0 of the TFFate architecture and testing suite
- Convert existing implementations of explicit momentum- and energy-conserving particle pushers to TFFate
- Begin implementation of semi-implicit algorithms, such as that developed by Lapenta, et. al. [5]
- Implementation of fully implicit algorithms, such as those by Chen, et. al. [6]
- Investigation of long-time-scale energy conservation
- Investigation of methods allowing for under-resolving of the cyclotron frequency

References

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