Decide how to handle multisim with modular simulator

GROMACS 2020 uses the legacy code path for all multisims. This includes replica exchange, ensemble restraints, and AWH. It remains to be decided at which level multisim should happen - does it need to be deeply incorporated in the simulator level (as in the legacy implementation), or could (most of) the functionality live outside of the simulator level and communicate via some type of API?

Related issues:
Related to GROMACS - Feature #3379: C++ API for simulation input and output

History
#1 - 03/11/2020 06:42 AM - Pascal Merz
- Description updated

#2 - 03/11/2020 11:53 AM - Eric Irgang
- Related to Feature #3379: C++ API for simulation input and output added