IP_6 Ion Simulation Planning Summary

October 21, 2025

1 Methodology

All estimates are derived from the historical IP_6 production runs in `ip6-run/process`. The workflow executed proceeds as follows:

1. **Density benchmark.** For every available reference run we read the solvated coordinate file to obtain the box volume V_{ref} and atom count N_{ref}. The median atomic number density is
$$\rho_{\text{med}} = \text{median}\left(\frac{N_{\text{ref}}}{V_{\text{ref}}}\right). \tag{1}$$

2. **Performance benchmark.** From each production log we extract the reported performance in ns/day[1] and form the product $k = (\text{ns/day}) \times N_{\text{ref}}$. The median of these values, k_{med}, captures the empirical throughput per atom.

3. **Ion targets.** The positive ion count N_+ is read from the project configuration of the selected microstate (default: IP_010101). Neutrality constraints are enforced by adjusting N_+ to the smallest value compatible with the solute charge and anion valence. In practice, this adjustment only increases N_+ when the requested cation has lower valence than the reference (e.g., $Ca^{2+} \to Na^+$); otherwise N_+ is unchanged. The corresponding negative ion count can be computed from charge balance.

4. **Box sizing.** For a desired molar concentration c ($\text{mol}\,\text{L}^{-1}$) we obtain the required solvent volume
$$V = \frac{N_+/N_{\text{A}}}{c} \times 10^{24}\ \text{nm}^3, \tag{2}$$
where N_{A} is Avogadro's number. For the cubic simulation cell this converts to an edge length $L = V^{1/3}$.

5. **Atom count estimate.** The total number of atoms expected for the target concentration is approximated by
$$N_{\text{atoms}} = \rho_{\text{med}} \times V. \tag{3}$$

6. **Wall-clock time.** The projected throughput is $\text{ns/day} = k_{\text{med}}/N_{\text{atoms}}$, hence the median wall-clock duration for a production length t_{sim} (ns) is
$$T_{\text{wall}} = \frac{t_{\text{sim}}}{\text{ns/day}} = 24 \times \frac{t_{\text{sim}}}{k_{\text{med}}/N_{\text{atoms}}}\ \text{hours}. \tag{4}$$
Slow and fast quartiles are generated in the same manner using the 25^{th} and 75^{th} percentiles of k.

[1] Typical values are around 150 ns/day for a concentration of 150 mM and a number of positive monovalent cations N+ = 12.

7. **Water-model scaling.** All benchmarks were carried out with TIP3P. For TIP4P/2005 we apply a conservative 33% overhead, i.e.,

$$T_{\text{wall}}^{(\text{TIP4P/2005})} = \frac{4}{3} T_{\text{wall}}^{(\text{TIP3P})}. \tag{5}$$

Thus, we use the equality $N_{\text{atoms}}^{\text{target}} \times (\text{ns/day})^{\text{target}} = N_{\text{atoms}}^{\text{ref}} \times (\text{ns/day})^{\text{ref}} = \text{const.}$ to scale wall-clock times for different system sizes.

2 Typical Wall-clock Estimates (default settings)

All simulations listed below assume IP_010101[2], a production length of 100.000 ns, temperature 310.000 K, and neutrality relative to the default ion counts. The table reports the median ("typical") wall-clock time for each ion, concentration, and water model combination.

Ion	Water model	Conc. (mM)	Box edge (nm)	N_{atoms}	Wall time (h)	Wall time (d)
Ca^{2+}	TIP3P	1.0	27.1	1.946×10^6	2.4×10^3	100.8
Ca^{2+}	TIP4P/2005	1.0	27.1	1.946×10^6	3.2×10^3	134.4
Ca^{2+}	TIP3P	2.0	21.5	9.728×10^5	1.2×10^3	50.4
Ca^{2+}	TIP4P/2005	2.0	21.5	9.728×10^5	1.6×10^3	67.2
Ca^{2+}	TIP3P	10.0	12.6	1.946×10^5	2.4×10^2	10.1
Ca^{2+}	TIP4P/2005	10.0	12.6	1.946×10^5	3.2×10^2	13.4
Mg^{2+}	TIP3P	0.5	34.2	3.891×10^6	4.8×10^3	201.6
Mg^{2+}	TIP4P/2005	0.5	34.2	3.891×10^6	6.5×10^3	268.8
Mg^{2+}	TIP3P	1.0	27.1	1.946×10^6	2.4×10^3	100.8
Mg^{2+}	TIP4P/2005	1.0	27.1	1.946×10^6	3.2×10^3	134.4
Mg^{2+}	TIP3P	10.0	12.6	1.946×10^5	2.4×10^2	10.1
Mg^{2+}	TIP4P/2005	10.0	12.6	1.946×10^5	3.2×10^2	13.4
Na^{+}	TIP3P	10.0	12.6	1.946×10^5	2.4×10^2	10.1
Na^{+}	TIP4P/2005	10.0	12.6	1.946×10^5	3.2×10^2	13.4
Na^{+}	TIP3P	140.0	5.2	1.390×10^4	1.7×10^1	0.7
Na^{+}	TIP4P/2005	140.0	5.2	1.390×10^4	2.3×10^1	1.0
Na^{+}	TIP3P	300.0	4.1	6.486×10^3	8.1	0.3
Na^{+}	TIP4P/2005	300.0	4.1	6.486×10^3	1.1×10^1	0.5

Table 1: Median wall-clock times for the default 18-run matrix (here the cation target was fixed to $N_+ = 12$).

The cumulative median wall-clock demand for the default plan is:

$$T_{\text{TIP3P}} = 1.2 \times 10^4 \text{ h } (\approx 4.9 \times 10^2 \text{ d}),$$
$$T_{\text{TIP4P/2005}} = 1.6 \times 10^4 \text{ h } (\approx 6.5 \times 10^2 \text{ d}),$$
$$T_{\text{combined}} = 2.7 \times 10^4 \text{ h } (\approx 1.1 \times 10^3 \text{ d}).$$

[2]Note, the selected microstate only supplies the solute charge, default N+, and box type.